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New advances in coal structure model

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ABSTRACT

Although human beings have come to understand and utilize coal for a very long history, no theoretical breakthrough in the study of coal structure has been made, which still needs continuous efforts of coal chemical workers. Based on the viewpoint of 'vague/clear', the species classification and accurate analysis on coal were conducted by using the natural clustering all-component separation method. A more systematic and detailed coal embedded structure model theory which is suitable for coal of all ranks was developed from the previous one and a more complete theoretical system about the component and structure of coal was constructed. The whole establishment process of the theory was summarized and some of the main support data and analysis test results, including TEM, AFM, FTIR, GC/MS, MALDI/TOF/MS, DART/MSD, fractal analysis and so on were provided. The coal embedded structure theory fully considers both the identity and the particularity of all-rank coal, reflects the coal component and structure in the full range of coal rank, solves the systematic cognitive problem of coal component and structure on macro and micro level, and provides a valuable and meaningful theoretical approach for the coal processing and conversion technology.

1. Introduction

Coal has a long history of discovery. In China, coal was known and used at the Neolithic period as early as 6000–7000 years ago. The history of utilizing coal was definitely recorded in the literature (Shan Hai Jing) which was over 3000 years ago [1]. Coal was used for combustion at the earliest. The technology of iron refining by using coal had matured in 266–420 at Jin dynasty, and it had begun to use coke derived from coal for iron refining in 960–1279 at Song dynasty [2]. Coal has obtained unprecedented development as a fuel power and as a raw material of coke since the industrial revolution in 18th century and the subsequent appearance of electric light. The first coal gasifier was built in 1832, and the first industrial process for water gas was successfully developed in 1875. The idea of F-T synthesis of liquid hydrocarbons and the concept of coal direct hydrogenation were proposed in 1913. The direct liquefaction pilot plant was completed in 1921, and the first trial of F-T synthesis was published in 1923. The first coal underground gasification test was conducted in 1933 [3]. After that till now, the technologies of coal utilization are developing continually. In particular, the new clean, efficient and comprehensive technologies such as the integrated gasification combined cycle (IGCC) power generation [4], the coal gasification polygeneration [5] and the coal staged utilization [6] which attracted great concern have obtained development and implementation. However, the foundation and origin of these technologies are all within the previously several aspects of the original creation, which are called burning, carbonization, gasification, direct liquefaction and indirect liquefaction. That is to say, although coal has been a major energy source for the whole human beings (coal was almost the only energy source before the extensive use of oil in the 1950s) and the metallurgical industry, the utilization of coal was limited to the improvement of above several methods and the development of the related downstream products. There is no new breakthrough for the idea innovation derived from origin and method innovation.

On the other hand, structure determines property, which reflects structure and determines application. However, the understanding of coal structure is very difficult. The reason is due to the highly complex solid characteristics, composition and structure of coal, and non-solubility of most components. In addition, imprisoned by the molecular structure idea in chemical theory, researchers always wanted to use one or several molecular structures to describe the complex coal structure [7]. Although the statistical averaged structure of some large molecular components of coal by simulation has certain significance, the fact that it conflicts with the actual situation of coal cannot be avoided. Therefore, there has been a saying in the field of coal chemistry during the few decades: the study of coal structure is so difficult that no coherent

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understanding has come to a conclusion and no systematic theory and method system has been constructed.

The above two aspects were reflected by three classic and authoritative works, which were Chemistry of Coal Utilization compiled and revised by Lowry H H in 1945 and 1963, respectively [8,9], and Chemistry of Coal Utilization compiled by Elliott M A in 1981 [3]. They systematically summarized the research achievements and industrial applications in the fields of international coal chemistry, coal chemical engineering and coal processing before 1978. However, there has not been a systematic summary for the development after 1978. Although the latest summary of systematic work is in lack, the problem of the two aspects has not been changed yet.

Nowadays, despite the serious environmental problems caused by the massive use of coal, coal is used continually, and there is no sign of great reduction and cancellation in the near future. Yürüm Y compiled Clean Utilization of Coal: Coal Structure and Reactivity, Cleaning and Environmental Aspects, which was published by Kluwer Academic Publishers in 1992 [10]. The book was published again with the title of Clean Utilization of Coal by Springer in 2010 [11]. It indicated that people paid a lot of attention to the problem of clean and efficient use of coal and tried continually to solve it, especially hoped to solve the current prominent problems of coal utilization through the relations of structure and reactivity of coal [12]. The key point still lies in the deep cognition of coal structure.

In order to get the new cognition of coal structure on current basis, the traditional thought and method need to be broken through. The first thing is to have a correct guide on epistemology. Because the composition and structure of coal is a highly complex system, from the point of philosophy, the cognition of coal structure will be vaguer if it is described accurately, while the cognition of coal structure will be more accurate if it is described vaguely. In other words, the more you want to know about coal from each molecule, the less you will know about coal in a whole. In contrast, the more you understand each part and typical characteristics of coal components based on a relatively vague model from the whole point of view, the clearer you will know about the overall structure of coal. Therefore, the cognitive method of coal structure must be in a view of macroscopic and vague (not from each specific molecule). Our point is using the method of all-component separation to classify the complex system into different species. Then each species which is still complex could be analyzed for more details by vague method. Finally, the species could be unified into a large system of coal structure, aiming to solve the difficult problem of the systemic cognition of composition and structure of coal from a macro point of view. In this way, valuable and meaningful theoretical guidance will be given for the new development of coal processing and conversion technologies.

This method is called vague/clear conception for cognition of coal structure for the moment. The vagueness means that it inherits the traditional conceptual description of coal structure characteristics, such as structure unit, side chain, bridge bond, functional group and cross-linking. It does not deal with the structure of particular (every) macromolecule, and it won't use a molecular structure model to represent the averaged macromolecular structure of coal. The clearness means that it innovates to traditional classification/separation idea on the basis of inheritance, and a new method of separation of coal group components with natural clustering characteristic is invented creatively, which could clearly classify coal into different species. After the detailed classification, the structure cognition can be carried out. The characteristics of this method are clearness in vagueness and vagueness in clearness, which are helpful for the understanding of coal structure more systematically and comprehensively.

2. Separation of all group components of coal by natural clustering

In 1985, Iino found that the mixed solvents of N-methyl-2-pyrrolidone (NMP) and CS_2 had high solubility of more than 70% for certain bituminous coal [13], which was considered as a major breakthrough in coal science research. During the next 20 years, many coal chemists in the world conducted various experiments, such as the component and structure of coal extracts, synergy between solvents, the relationship between extraction rate and swelling rate, the influence of coal rank and petrographic components on the extraction rate, the effect of non-covalent bonds in coal and the effect of additives [14–19]. These researches raised the cognitive level of coal structure, and the representative achievement was the establishment of the concept of the associated structure model [20]. However, after 2005 there were fewer and fewer studies on coal mixed solvents, and only a few literatures were published [21–24].

On the basis of several years of research, the author made a great improvement to this method in 2004, which was multi-step back-extraction operation for the extraction liquid by CS_2/NMP mixed solvents [25]. The basic flow of this method is shown in Fig. 1.

Firstly, the pretreated coal samples of about 74 μm were extracted by CS_2/NMP mixed solvents. The insoluble residue was centrifuged as the first group component and called the heavy component (HC). Then deionized water used as back extractant was put into the extraction liquid and stirred. Three layers were generated after centrifugation. The lowest layer was the second group component and called the loose medium component (LMC). The middle layer solution was separated out, and extracted by the back extractant H_2O after CS_2 was evaporated. In this process, the solid asphaltic component was precipitated as the third group component, and called the dense medium component (DMC). The back extracted liquid during the two back extraction processes were mixed, and then the back extractant H_2O and the extractant NMP were evaporated through atmospheric and vacuum distillation, respectively. The fourth group component was obtained in this process, and called the light component (LC).

Both the extraction process and back-extraction process exist in above method, so it is called extraction and back-extraction method of coal. Except that the light component is obtained

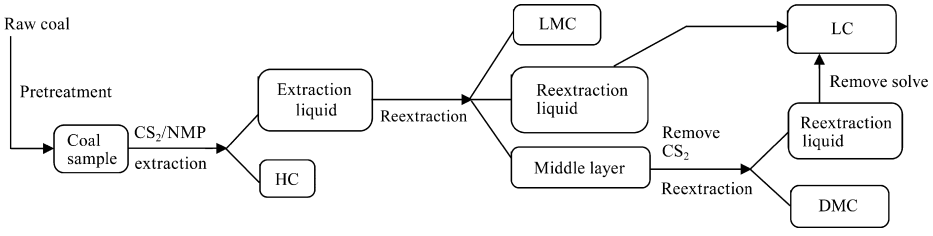

Fig. 1. Process flow diagram of coal all-group separation method.