Commun. Comput. Chem. Vol.**2**, No.**1**, pp.1-8
doi: 10.4208/cicc.2014.v2n1.1 March 2014

COMMUNICATION

A Post-Processing Program for ReaxFF Simulation of Chemical Structural Model of Coal

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Received 28 Feb 2014; Accepted (in revised version) 15 March 2014

Abstract: A post-processing program for ReaxFF simulation of chemical structural model of coal is designed by C++ codes. The results of tests for the program show good agreements with known coal chemistry. The distributions of particular molecules, hydrogen bonds, π-π stacking interactions and cleavage/cross-linking reactions can be summarized by this program. These informations are hard to directly obtained from the ReaxFF results for such a complex system as coal. Furthermore, this program could find out the specific sites of a noncolvant interactions and cleavage/cross-linking reactions, and refine the corresponding molecular geometries. This is helpful to understand the thermal reaction mechanisms of coal.

AMS subject classifications: 68U05, 68U07

Key words: Chemical Structural Model, Coal, ReaxFF, Intermolecular Interaction

Coal is the primary energy resource in China. It takes nearly 70% of our total energy consumption [1]. In order to make full use of coal, coal reactions are widely performed, such as coal pyrolysis [2], liquefaction [3], gasification [4], etc. These reactions are closely related to structures of coal samples. From the beginning of the 21st century, more and more researchers have begun to study chemical structural models of coal [5], which could represent the statistical structures of corresponding coal samples. So far, more than 130 kinds of chemical structures have been proposed. Based on these models, the thermal reactions and properties of coal can be simulated by molecular dynamics simulation or quantum chemical calculations [6].

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Reactive Force Field (ReaxFF) molecular dynamics simulation is a method developed by van Duin [7]. With this method, van Duin examined the structural transformations and chemical processes associated with the coal char at very high temperatures (3000~4000 K) [8]. Since then, the ReaxFF has been used to study coal reactions. E. Salmon used the ReaxFF method to reproduce the thermal decomposition of the Morwell brown coal [9]. X. X. Li and L. Guo have performed coal pyrolysis at 1000~2000 K by ReaxFF simulation [10]. They obtained the sequence of gas generation and product profiles. So, the ReaxFF simulation has been successfully used to explain thermal reactions of coal.

However, our previous work has identified that thermal reactions system of coal in ReaxFF simulation is much too complex at high temperatures. In this system, there are many non-covalent interactions between molecular fragments, such as hydrogen bond and π-π stacking interaction. Hundreds of molecules could react with each other and produce new molecules at every time step. Furthermore, it also includes thousands of coupled reaction pathways, involving cleavage reaction and cross-linking reaction. All of the above simulation results are necessary for the study of the thermal reactions of coal. But they are hardly counted by manual work. In this communication, we describe a new designed post-processing program for ReaxFF simulation of chemical structural model of coal by C++ codes. In this program, we can easily count the number of molecules and intra-/inter-molecular interactions at every time point in the ReaxFF simulation. The geometries of reactants and products in the cleavage or cross-linking reactions could also be obtained by this program, which is difficult to be directly observed in so many atoms.

In order to study the geometrical changes of atoms and molecules in the program, an appropriate data structure is needed to represent each atom and molecule, and then the chemical reaction process. Our study on the chemical reactions of coal is focused on the ReaxFF simulation system containing C, H and O elements.

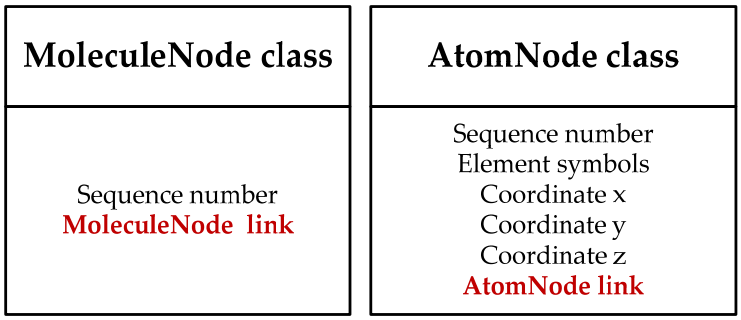

Figure 1: The molecular and atomic link node class structure.