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Quantum Chemistry-Based Molecular Mechanisms and Ageing Resistance Improvement Techniques for Asphalt

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Abstract

Asphalt is a common building material for roads because it is a crucial adhesive. Asphalt ages through a series of aging processes, including volatilization, oxidation, and polymerization, which cause it to become hard and brittle under the influence of high temperature, oxygen, water, ultraviolet rays, and other factors. Pavement damage such as thermal crack, fatigue crack, and cohesion failure accelerate with asphalt aging, significantly shortening the pavement's service life. During the asphalt aging process, the most important reaction is oxidation. To improve asphalt's resistance to aging, it is essential to comprehend the oxidation reaction mechanism.

Keywords: Quantum chemistry • Asphalt • Electrophilicity

Introduction

To explain the oxidation reaction mechanism, researchers have divided asphalt into saturates, aromatics, resins, and asphaltenes (SARA) fractions and evaluated changes in the proportion of these fractions or the behavior of various functional groups in the asphalt. Petersen, others tested the amount of ketones produced by aging to determine the oxidation reactivity of fractions and demonstrated SARA's oxidation reactivity. The decrease in aromatics, the increase in asphaltenes, and the potential increase or decrease in resins are all due to the molecules of aromatics, resins, and asphaltenes being more polar than those of saturates and being more prone to oxidation to form polar functional groups [1].

Literature Review

Oxidation mostly results in the formation of ketones, aldehydes, anhydrides, carboxylic acids, and sulfoxides as functional groups. More than 80% of these groups are made up of ketones and sulfoxides. Sulfoxide is regarded as the predominant oxidation product in short-term aging, whereas ketone is regarded as the predominant oxidation product in long-term aging due to its faster formation rate. The benzylic carbon site is most likely where ketones are made, followed by the tertiary, secondary, and primary alkyl sites. Asphalt has numerous ketones and a lot of benzyl sites. The oxidation results in the formation of stable dicarboxylic acid anhydrides in some molecules that have two adjacent benzyl carbons. The above research qualitatively clarified SARA's oxidation reactivity, as well as the oxidation-induced changes in SARA's content and functional group [2,3].

However, experiments are unable to accurately test the molecular oxidation site and reactivity due to the asphalt's complex composition. Experiments also cannot accurately test the oxidation reaction process because it involves numerous steps. To address the aforementioned issue, it is necessary to investigate the mechanism of the oxidation reaction using theoretical calculations, used aging theory to introduce ketones and sulfoxides into the original asphalt molecules to create molecular models of aged asphalt. After that, the researchers determined the effect of asphalt aging on its properties by comparing the original and aged asphalt in terms of asphaltene aggregation, molecular diffusion behavior, and surface free energy using MD simulation [4].

Discussion

However, the author's subjective views heavily influence the aging theory-based aged asphalt model, resulting in randomness. Reactive force field (ReaxFF) molecular dynamics can also predict the oxidation products and simulate the asphalt oxidation reaction as it ages. Quantum chemistry calculations of reactants, products, high-energy intermediates, and transition states are used to parameterize ReaxFF. The quantum chemistry-derived parameter set determines the accuracy of ReaxFF MD. There are no ReaxFF parameter sets for asphalt because fitting parameters require a lot of computational power. Asphalt research typically makes use of the ReaxFF parameter sets of low molecular weight hydrocarbons. The application of these parameter sets to asphalt, on the other hand, may result in an inaccurate estimation of the impact of intramolecular interactions on chemical reactions due to the substance's large molecules. In addition, the ReaxFF-derived oxidation products are typically generated in a high-temperature simulation above 1000 K, which does not correspond to the actual aging conditions, saving time in the simulation [5].

Quantum chemistry (QC) is an effective method for analyzing atomic-scale chemical reaction mechanisms. Numerous materials' reactivity, reaction sites, reaction pathways, and reaction rate can all be predicted using this method. The evaluation of various methods for predicting the electrophilicity and nucleophilicity of organic molecules is one application. By looking at how energy changes during reaction processes, researchers also predicted reaction pathways and rates. Liu and Edwards et al.'s organic oxidation reactions compared the rates of oxyradical decomposition on various structures and the oxidation pathways and rates of polycyclic aromatic hydrocarbons (PAHs) at combustion temperatures. Quantum chemistry offers significant advantages for studying chemical reaction mechanisms, as the preceding research demonstrates [6,7].

The study of additives' effects on asphalt properties has been the primary focus of QC's asphalt application, and its use in the investigation of the asphalt oxidation reaction mechanism is limited. Pan and co. compared lignin's oxidation reactivity with hydrocarbons to determine its antioxidant effect and discovered that lignins could enhance the antioxidant properties of hydrocarbon molecules with larger HOMO–LUMO gaps. Pahlavan and team investigated the interaction and came to the conclusion that the bio-modifiers could lessen the effect of oxidation-induced polar substitutions on the aged asphalt [8].

Mousavi, others analyzed the chain of reactions that occurred between rubber molecules and bio-modifiers and discovered that bio-modifiers increased the surface polarity of rubber, which in turn increased the interaction between rubber and asphalt and decreased phase separation in rubberized asphalt. Hu

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and co. studied the change in free energy caused by an asphaltene molecule's oxidation reaction and discovered that aromatization has the lowest free energy barrier, followed by the formation of oxygen-containing groups and the homolysis process. The study ignored the variety of asphaltene molecules and concentrated on a single molecule of asphaltene. In addition, the oxidation reactivity, pathway, and rate of asphalt molecules were not studied, making it difficult to accurately improve asphalt's aging resistance [9].

The oxidation reaction mechanisms of asphalt molecules were examined using QC in this study. The electrostatic potential, average local ionization energy, and Fukui function were used to make predictions about the oxidation sites on asphalt molecules. Local softness was used to measure molecules' oxidation reactivity. Transition state search, intrinsic reaction coordinate, vibrational frequency, and single-energy calculations were used to investigate the oxidative reaction pathways and free energy changes. The Eyring equation and the changes in free energy were used to calculate the reaction rate. The molecular models of aged asphalt and optimization strategies to increase asphalt's aging resistance were proposed on this foundation. The aging mechanism of asphalt is further revealed in this study, which has the potential to enhance asphalt's aging resistance and promote pavement sustainability. In addition, the molecular models of aged asphalt are established, laying the groundwork for molecular-scale research into its structure and properties [10].

Conclusion

The aged asphalt molecular models. According to Peterson et al.'s experimental research conclusion, the oxidized molecular model constructed in this paper has one oxygen-containing group on average, as shown in the figure. A series of high-precision quantum chemistry calculations and consideration of reaction rates under actual aging conditions determine the molecular models. ensuring that the model is as rational and accurate as possible. However, due to the computational requirements of quantum chemistry, the oxidation of molecular clusters is ignored in this study, which focuses solely on the reaction of single molecules with oxygen or free radicals. molecular dynamics or reaction kinetics will be used in subsequent studies to gain a deeper understanding of the asphalt oxidation mechanism at the molecular scale. For ReaxFF molecular dynamics and reaction kinetics research, this paper's calculation results will provide important input parameters and preliminary exploration parameters.

Acknowledgement

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Conflict of Interest

None.

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