

Review Article

The State-of-the-Art Review on Molecular Dynamics Simulation of Asphalt Binder

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Asphalt pavement has been widely used in the world. As the main components of asphalt pavement, the asphalt binder is crucial to the service performance and life of the road. In the past decades, numerous studies were conducted on technical performance, aging, and modification of the asphalt binder. With the development of modern technology, it was discovered that the microscopic properties, aging mechanism, and modification mechanism of the asphalt binder affect the macroscopic performance of asphalt pavement significantly. As a new emerging powerful numerical tool, the molecular dynamics (MD) simulation has been developed to study the asphalt binder material from a micro perspective. Based on the previous studies, some average asphalt binder models, fractional asphalt binder models, aged asphalt binder models, and modifier models were proposed by many researchers, which have made remarkable progress in asphalt studies; the microproperties, aging mechanism, and modification mechanism of the asphalt binder can also be analyzed using the MD simulation. Overall, the state-of-the-art review provides a comprehensive view for the readers to better understand the development, establishment, and application of the asphalt molecular model.

1. Background and Introduction

With the rapid development of modern transportation in the world, the asphalt pavement structure has become one of the most preferred structures of highways due to its advantages for comfortable driving and fast traffic opening [1]. Since the asphalt binder is the main bonding material for the road, its properties are crucial to the service performance and service life of the pavement, that is, the quality of the pavement in service life depends largely on the quality of the asphalt binder [2, 3]. So far, many scholars have studied the technical performance of asphalt [4–20], including aging resistance [21–25], adhesion property [26–28] self-healing behavior [29–32], fatigue-resistance performance [33–39],

modified improvement [40–47], and so on. However, most of these investigations are based on the macroscale experiments including the penetration test, ductility test, softening point test, DSR, and BBR. In a recent investigation on asphalt microproperties, it was discovered that the microscopic properties of asphalt significantly affect the macroscopic properties. Because the asphalt microproperties have a strong relationship with the chemical composition, which is considered to be the main reason for its microscopic properties, it has attracted the attention of many scholars. Since the asphalt binder itself is a by-product of the petrol industry, there exists more than a million chemical compositions in the asphalt binder. Therefore, it is necessary to simplify and separate the asphalt binder into a few fractions

for the basic investigation. The mainstream method separates the asphalt binder into aliphatics, naphthene aromatics, polar aromatics, and asphaltenes according to different polarities created by Corbett [48]. With this method, the chemical properties of each fraction can be studied, and some chemical structures are proposed to explain the mechanism of properties of the asphalt binder at a molecular scale.

However, the chemical composition separation can only study the asphalt binder from static state and cannot dynamically describe the chemical structure, whereas a molecular dynamics (MD) simulation can reflect the thermodynamic behaviors of asphalt molecules and has therefore been developed. The MD simulation was firstly employed in biology in terms of protein molecules and nutrition; then it was developed by the field of petroleum to study the properties of petroleum; later, in the asphalt industry, the MD simulation was also developed to solve many problems at microscale [49, 50]. Greenfield has made significant contributions in this area [51–53]. The research progress is shown in Figure 1.

MD simulation is conducted at microscale to analyze the main physical and mechanical properties of the asphalt binder based on the molecular interaction and local dynamics of particles. Some research studies in terms of MD application were investigated by us: the effect of wasting cooking oil on the macro- and microproperties of the asphalt binder, nanocracking under external loading conditions in the asphalt binder, and hardening effect on asphalt binder during the aging process as well as the effect of paraffin on the microproperties of the asphalt binder [49, 54–58]. In this study, we would like to describe the development status and some applications of this technology; some specific research of asphalt binder models is also described in this paper. The main properties of the binder including density, glass transition temperature, diffusion coefficient, adhesion, self-healing behavior, and so on can be calculated. The objective of this paper is to introduce the state-of-the-art research process on the molecular models of the asphalt binder, as well as the applications of MD simulation, based on which further research on the asphalt microscopic properties investigation at microscale is expected to be conducted. A schematic view of the MD simulation in the asphalt binder is shown in Figure 2.

2. Chemistry and Structure of Asphalt Binder and Fractions

2.1. Asphalt Binder Molecular Structure. To investigate the asphalt binder from a microscopic perspective, Jennings et al. [59] built eight average molecular structures for the core asphalt binders in the Strategic Highway Research Program (SHRP) (Figure 3). The physical properties of those core asphalt binders have been investigated by Pauli et al. [60], and an alicyclic sheet molecule was recommended to represent the asphalt binder. Based on their research results, the physical properties of those real asphalts were studied by the corresponding average models.

However, the asphalt binder consists of millions of kinds of original components [61]. To study the components in the asphalt binder in depth, the asphalt binder was separated

into aliphatics, naphthene aromatics, polar aromatics, and asphaltenes according to the Corbett method [48], which is a mainstream method in the field of crude oil. The four fractions have their own unique properties.

2.2. Chemical Composition. Based on previous research, the chemical structure of each fraction in the asphalt binder was investigated, and then reasonable microscopic structures for different asphalt binders were created to represent the asphalt binder accurately.

2.2.1. Aliphatics. At room temperature, aliphatics form a light-coloured liquid [48]. By means of the Fourier transform infrared spectroscopy (FTIR), it is known that there are different kinds of branching structures and some aliphatic chains in the aliphatics structure, almost all atoms and aromatic rings are nonpolar, and the average molar mass of aliphatics is 600 g/mol approximately [62].

The aliphatics is the fraction with the least polarity, and compared with the other fractions, the chemical properties of aliphatics is the most stable [63, 64]; oxidation or dehydrogenation reactions are difficult to carry out [65] because there is only a few polar atoms or aromatic rings on aliphatics [62]. In terms of chemical structure, n-docosane ($n\text{-C}_{22}\text{H}_{46}$) was chosen as a representative aliphatics by Kowalewski et al. [66]. Later, an aliphatic structure squalane was obtained from animal sources and plant; it can also be found in petroleum [67, 68]. In addition, another aliphatic structure hopane was derived from crude oils and biodegraded oil shales commonly, which were constituents of bacterial cell membranes [69]. These typical molecular structures for aliphatics are shown in Figure 4.

2.2.2. Naphthene Aromatics. At room temperature, naphthene aromatics are liquid with the colour yellow to red [48]. Compared with the aliphatics, naphthene aromatics behave more viscous at the room temperature. There are very few aliphatics with lightly condensed aromatic rings on their carbon skeleton, and the average molar mass of the fraction is about 800 g/mol [62]. In addition, previous research demonstrates that some naphthene aromatics have negative impacts on human health, such as impaired lung function in asthmatics, and is even the cause of cancer in laboratory animals [70].

The glass transition temperature (T_g) of naphthene aromatics is around -20°C , which is consistent with that of the bitumen parent; hence, at the same temperature, naphthene aromatics have a higher viscosity than the aliphatics due to its T_g [71, 72].

Some aromatic, naphthenic, and paraffinic compounds are in naphthene aromatics component [73]. 1,7-Dimethylnaphthalene was selected to represent naphthene aromatics [74]. The alkane/aromatic ratio of 1,7-dimethylnaphthalene is 16.7:83.3, which is different from the overall 58:42 balance [74]. There are some side chains and aromatic rings on the 1,7-dimethylnaphthalene, the number of which can make 1,7-dimethylnaphthalene intermediate between aliphatics and asphaltenes. Later, another structure of naphthene aromatics

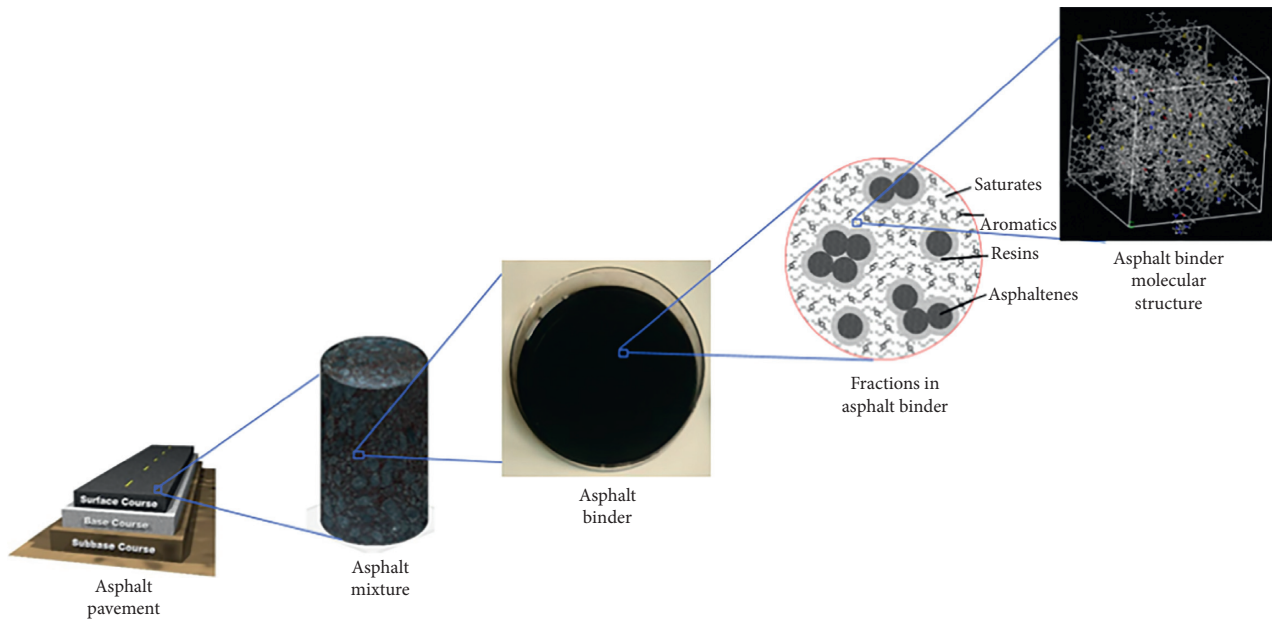


FIGURE 1: Asphalt research from macrolevel to microlevel.

called perhydrophenanthrene-naphthalene (PHPN) was proposed by Lira-Galeana and Hammami, which contained aromatic rings joined with naphthenic rings [75]. Simanzhenkov and Idem found that dioctyl-cyclohexane-naphthalene (DOCHN) can represent an average naphthene aromatic structure by means of n-d-M method; the DOCHN structure was consistent with the mass ratio of carbons on aromatics, naphthenes, and paraffins in crude oils, and its rationality was validated using some parameters, such as the measurements of refractive index, density, and molecular weight of the fraction [76]. So, naphthene aromatics can be represented by three kinds of molecular structures, which are shown in Figure 5.

2.2.3. Polar Aromatics. Polar aromatics form black-coloured solid at normal temperature [48], the molar mass of them is less than asphaltenes, but their composition is close [77]. The glass transition temperature of polar aromatics is still not confirmed [71, 72]. The typical structure of polar aromatics contains fused aromatic rings with 2–4 fused rings [62]. They are important for the stability of asphalt binder, because in asphalt binder, polar aromatics are a stabilizer for the asphaltenes [78].

Koots and Speight found that the composition of polar aromatics and asphaltenes were similar [77]. Pieri found that the polarity of polar aromatics could be larger than that of asphaltenes sometimes, although having less condensed aromatic rings [62]. Average polar aromatics molecule structures were built by Murgich et al. to analyze molecular recognition [79]. These structures derived from fresh water lacustrine source rocks were identified by Oldenburg et al. by means of gas chromatography-mass spectrometry (GC-MS) [69]. Koopmans et al. studied the alkylsulfide fraction of sedimentary rock samples and extracted a polar aromatics component thio-isorenieratane by means of gas chromatography

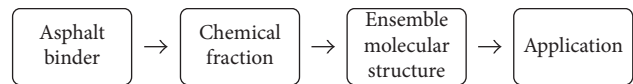


FIGURE 2: Schematic view of MD simulation in asphalt binder.

(GC) [80]; later, they identified another polar aromatics component trimethylbenzene-oxane in shale rocks using GC [81]. Then, benzobisbenzothiophene was identified in organic extractions from sedimentary rocks using GC-MC methods. Lira-Galeana and Hammami [75, 82] built average polar aromatics molecule structures containing two organic groups connected by sulfur elements. These typical molecular structures for polar aromatics are shown in Figure 6.

2.2.4. Asphaltenes. At room temperature, fraction asphaltenes are black powder [48]. They do not have any thermal transition up to 200°C [71]. Asphaltenes are defined as the fraction which is an insoluble part in *n*-heptane but soluble in toluene [84]. So a colloid model was proposed for the asphalt binder, in which asphaltenes are covered with polar aromatics and suspended in naphthene aromatics and an aliphatic medium [85]. The asphaltenes are crucial for the technical properties of the asphalt binder, so they are by far the most studied fraction in asphalt binders [86]. Their average molar mass is about 800–3500 g/mol [87, 88]. Furthermore, Van Hamme et al. found that there were many aromatic rings and aggregates in hydrocarbon solvents in asphaltenes [89]. Brandt et al. predicted that asphaltenes could stack in some solvents using thermodynamic modeling, and the maximum number of aggregated asphaltene molecules was five [90].

Pacheco-Sánchez et al. found that the number of asphaltene aggregation decreased as temperature increased

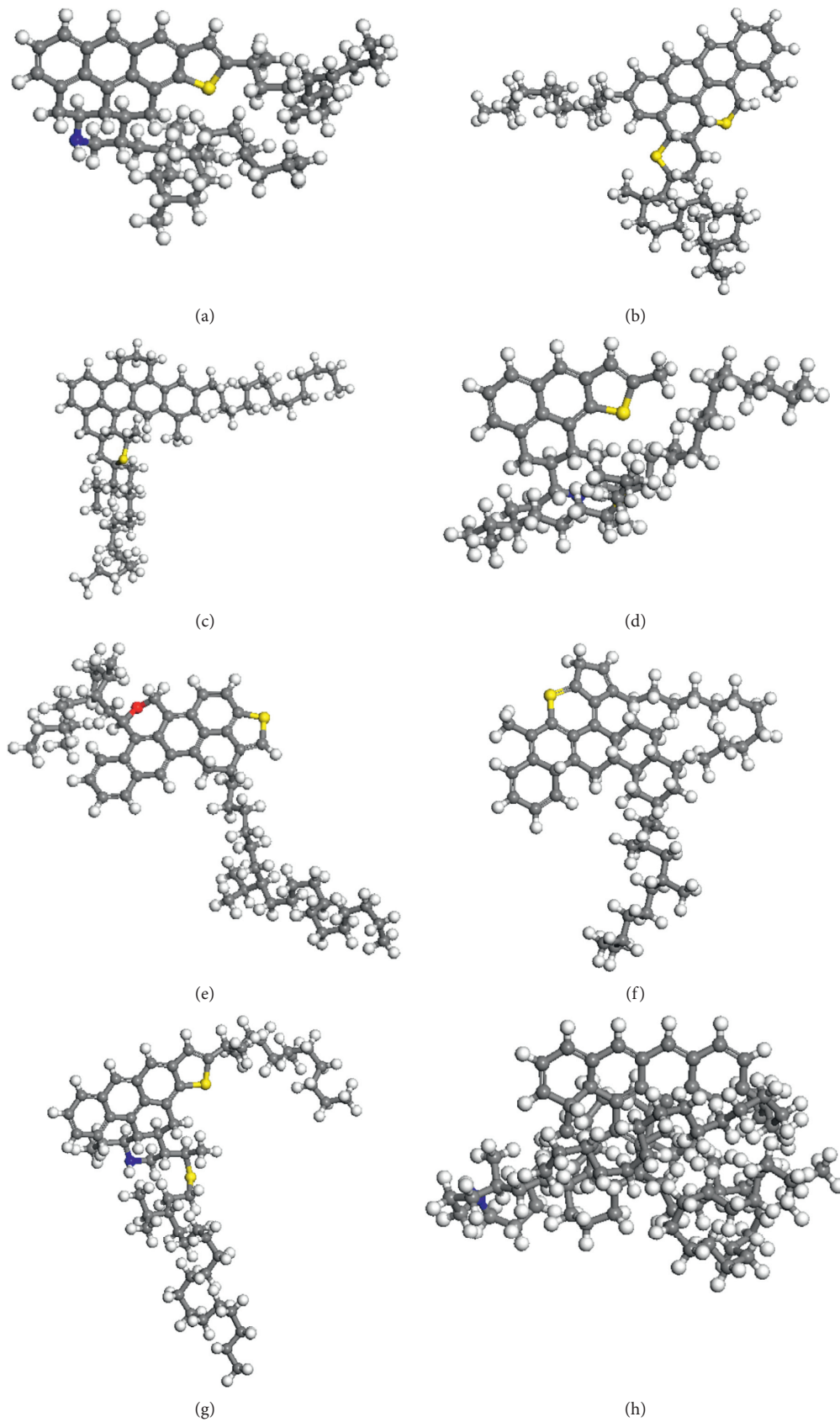


FIGURE 3: Average molecule for each of the SHRP binders [59]: (a) AAA-1, (b) AAB-1, (c) AAC-1, (d) AAD-1, (e) AAF-1, (f) AAG-1, (g) AAK-1, and (h) AAM-1.

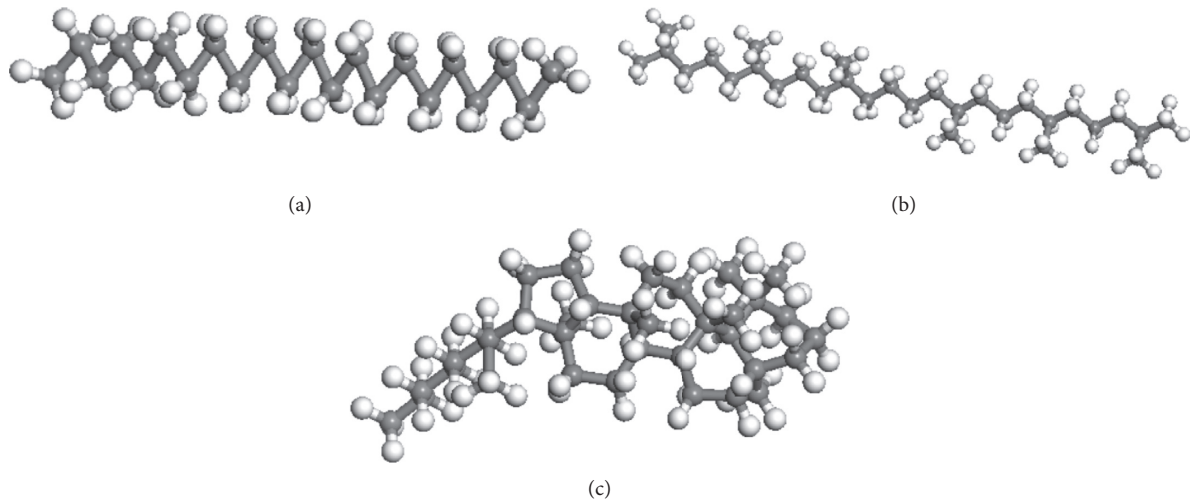


FIGURE 4: Typical molecular structures for aliphatics [33–35].

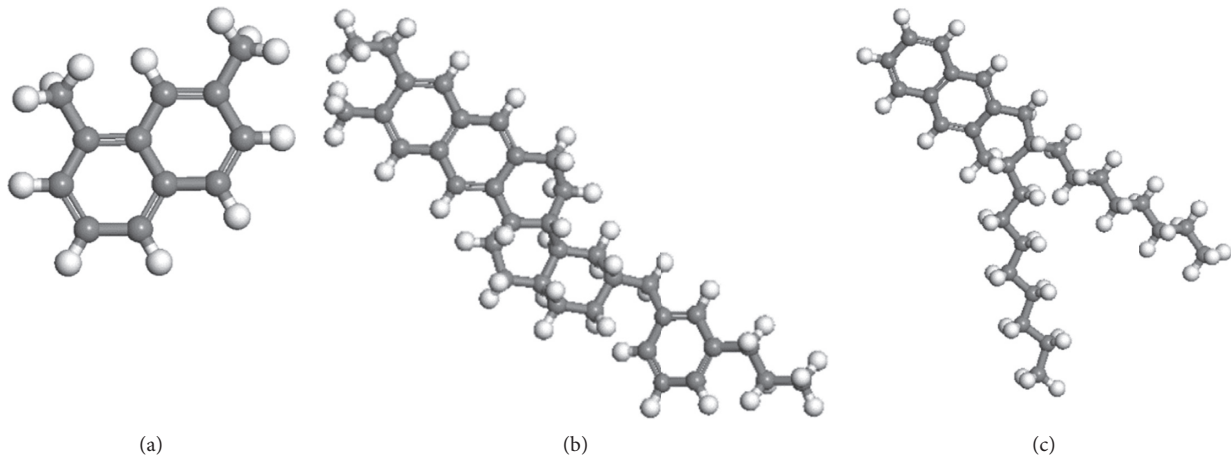


FIGURE 5: Typical molecular structures for naphthene aromatics [37, 38].

[91] and mostly the characteristics of crude oil determine the aggregate orientation [92]. Yen et al. investigated the structure of asphaltenes and found that the interlayer distance between aggregated asphaltene molecules was 3.5–3.8 Å using X-ray diffraction ($1 \text{ \AA} = 10^{-1} \text{ nm}$) [93].

Murgich et al. built an average chemical molecule structure for asphaltene to investigate the mechanism of asphaltene aggregation [79]. Artok et al. built several asphaltene chemical structures containing a moderate-size aromatic core with small branches based on experimental data [94]. Groenzin and Mullins [95] recommended more models with smaller aromatic core and much longer alkane side branches for asphaltene structures by means of fluorescence measurements.

Yen assumed that the asphaltene was composed of extensive condensation of aromatic rings [96]. Afterwards, Groenzin and Mullins proposed a kind of this structure with lower molecular molar weight based on spectroscopic studies. Compared with the structures proposed earlier [56],

this molecular structure was closer to the true asphaltene. Siskin et al. investigated different asphaltene from different production areas and their chemical properties and then proposed six average molecular structures for asphaltene [97]. Some typical asphaltene models are shown in Figure 7.

3. Molecular Model

3.1. Creation of Fractional Asphalt Binder Model. Based on the chemical structures of each fraction, some chemical models of the asphalt binder are proposed.

3.1.1. Three-Component Asphalt Binder Model. In the field of asphalt binder materials, two asphalt binder models were created by Zhang and Greenfield to investigate the properties of asphalt binders [100–102], one of which contained 5 asphaltene proposed by Artok et al. [94], 27 1,7-dimethylnaphthalene, and 41 $n\text{-C}_{22}$ molecules, and the other of which consisted of 5 asphaltene proposed by Groenzin and

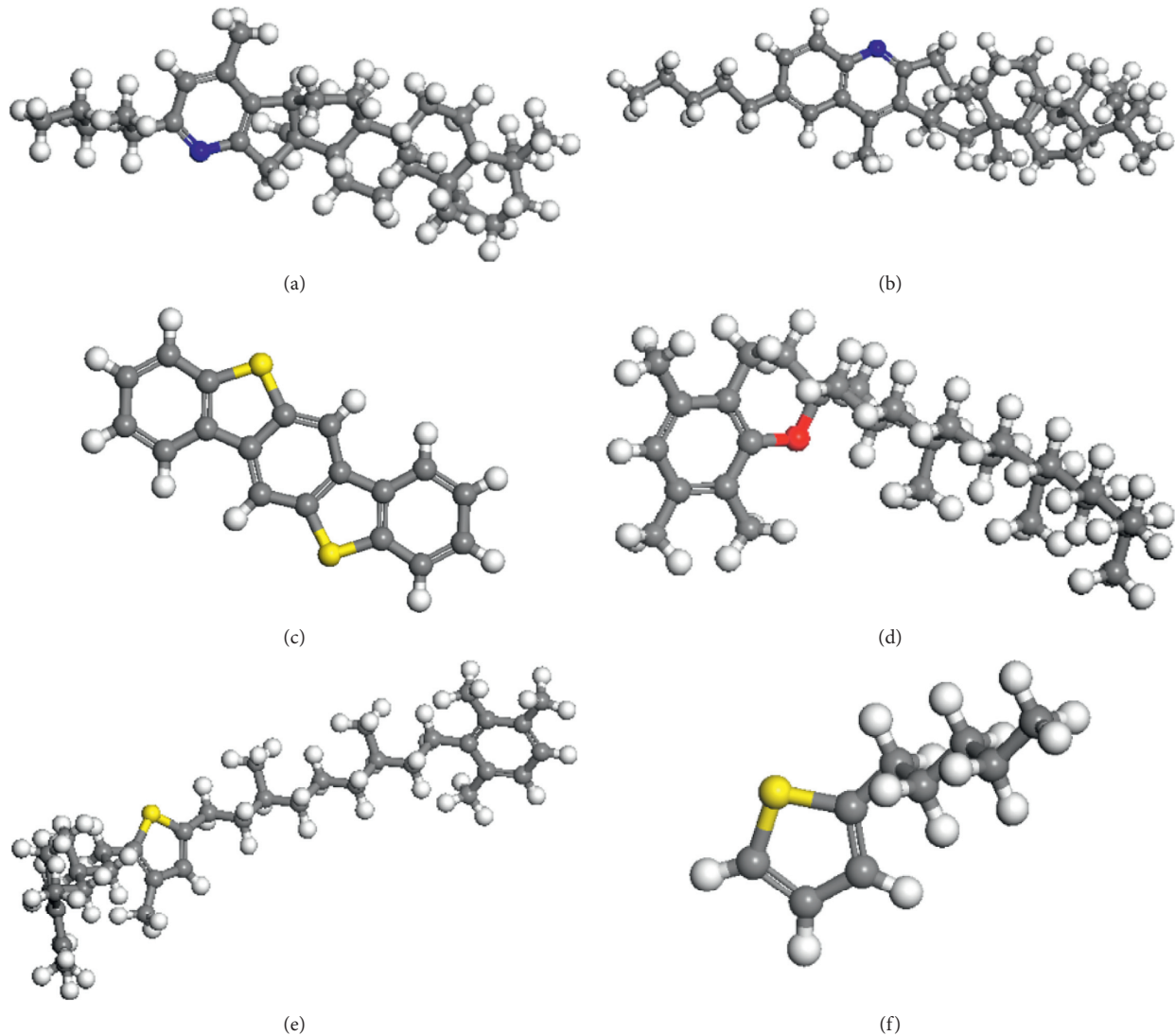


FIGURE 6: Typical molecular structures for polar aromatics [35, 40, 42, 43, 83].

Mullins [95], 30 1,7-dimethylnaphthalene, and 45 n-C₂₂ molecules. The two asphalt binder models consist of 21% asphaltenes and 59–60% aliphatics, which is consistent with the content of the total C/H ratio reported for a real asphalt [74, 103].

These asphalt binder models have been used in some research: the effect of fractions on the micromechanical behaviors of the asphalt binder [49], the influence of SBS modifier on molecular agglomeration behavior of the asphalt binder using the radial distribution function data [104], the micromechanism of self-healing behavior of the asphalt binder using the morphology of the molecules in the asphalt binder [105], and the interactive response between the asphalt binder and different aggregate [106].

These asphalt binder models were the first molecular model for the asphalt binder, which helped researchers solve a lot of mechanism problems from a micro perspective, and the models had landmark meaning. However, only three fractions exist in the model; there are possibilities for improvement.

3.1.2. Twelve-Component Asphalt Binder Model. With the development of molecular simulation technology, more accurate asphalt binder models were established. Li and Greenfield [99] created three kinds of asphalt binder systems (AAA-1, AAK-1, and AAM-1) with 12 chemical components according to the ratio of the four fractions, mass percentage of element of carbon, hydrogen, oxygen, nitrogen and sulfur, atomic H/C ratio, and aromatic and aliphatic percentage of carbon and hydrogen, and they are the widely used asphalt binder models. Compared with the previous asphalt binder models, these models with 12 components are more reasonable and closer to the nature of the real asphalt binder. The only disadvantage is that these models cannot represent the other kinds of asphalt binder.

The twelve-component asphalt binder model was used for some scientific issue: the cohesive and adhesive properties of asphalt binder, including the adhesion between asphalt binder and aggregate; the influence of moisture on their adhesive property [107]; the mechanical performance and modified modification of the asphalt binder with

different waste cooking oil contents [57]; and the oxidative aging effect of asphalt binder, including the influence of aging on the self-healing behavior and moisture damage behavior of asphalt [108].

3.1.3. Aged Asphalt Binder Model. Based on the asphalt binder models mentioned above, some aged asphalt binder models were proposed. Generally, the aged asphalt binder model can be divided into two ways to characterize it. The first approach is to adjust the proportion of asphaltene structures [109], which is consistent with the increases of asphaltene content after aging. However, it is not taken into account that some oxidation reaction occurs during the aging procedure. So another approach has been proposed by Yao et al. [110] and Xu and Wang [108]. Yao added a carboxylic acid group on the asphaltene molecule to represent aged asphaltene. Xu and Wang added some oxygen atoms on the asphaltene, naphthalene aromatics, and polar aromatic molecular structures, and the molecular structure of aliphatics remained unchanged, because the content of polar atoms and aromatic rings was too small [108].

3.2. Creation of Modifier Model. In recent years, the modified asphalt binder has been used widely in the pavement area due to its excellent technical performance. So it is necessary to investigate the modifier for the asphalt binder.

3.2.1. Polymer. Currently, the simulated modifier in the asphalt binder is SBS, graphene, and carbon nanotubes. Ding et al. studied two kinds of SBS modifiers in the asphalt binder and based on the radial distribution function (RDF) data to analyze the impact of these two kinds of SBS on the molecular agglomeration state of asphalt binders [104].

Zhang and Greenfield [101] investigated the effects of polystyrene modification on properties and the microstructure of asphalt system models because polystyrene is part of the common modifier SBS.

3.2.2. Graphene and Carbon Nanotubes. Yao et al. compared the two models of the asphalt binder with exfoliated graphite nanoplatelets (xGNP) and control asphalt binder by means of MD simulation to study the physical and thermal properties of the xGNP-modified asphalt binder [110].

A comparative study was employed to study the effects of graphene and carbon nanotubes (CNTs) on the mechanical and thermal properties of the asphalt binder using molecular simulations, and in experiments by Zhou et al. they found that the excess graphene in modified asphalt remained as aggregated particles, while most carbon nanotubes were dispersed in modified asphalt [111].

3.2.3. Rejuvenator. The effect of different rejuvenators on recycled asphalt mixtures was investigated using MD simulation by Ding et al. [109], and they found that the interdiffusion rate between asphalt binders at different aging stages could be accelerated to the maximum rate when

adding a rejuvenator into the aged binder, which can improve the efficiency of recycling.

Xiao et al. investigated the diffusion behavior of two different rejuvenators in an aged asphalt binder at the molecular scale. Meanwhile, dynamic shear rheometer (DSR) was employed to determine the recovery influence of aged bitumen resulting from rejuvenators [112]. The test results validated the accuracy of the model simulation results and indicated that the aging state of asphalt binders greatly influenced the rejuvenating effect [113].

Some typical molecular structures for modifier are shown in Figure 8.

4. Applications

4.1. Nanocracking Behavior. Fatigue damage is the main distress in asphalt pavement; it influences the fatigue life of pavement significantly [114–119], and the fatigue damage gradually generates with the appearance and development of macro- and microcracks under the loading of vehicle and temperature [120]. In order to study the fundamental asphalt binder material properties for the crack, a pair of big enough-opposing forces is applied on the molecular boundaries, then the molecules are pulled by an external force, and a crack appearance can be observed. The stress state of the molecules in an asphalt binder model can be observed with the MD simulation; in addition, the process of molecules being pulled apart can also be observed by some visual software. Hou et al. studied the initiation and propagation of crack in asphalt binder applying tension force on the molecular boundaries, and they found that the natural distribution of atoms at microscale would affect the intrinsic defects and further influence initiation and propagation of crack in the asphalt binder [58]. Nishimura and Miyazaki have used the MD simulation of a-Fe to investigate the mechanical behaviors under cyclic loading from a micro perspective. They made a crack on the boundary of a 2D material, then cyclic loading was applied to the system 12 times, and generation of several vacancies around the crack tip and the crack propagation under cyclic loading were observed [121]. Shang and Kitamura studied the onset of fracture at the free edges of bimaterial interfaces; crack initiation at interface edge models with different contact angle were created to clarify the relationship between crack initiation, contact angle, and maximum stresses [122]. This investigation is meaningful for the research of adhesion between the aggregate and asphalt binder.

4.2. Tire-Aggregate Friction. The tire-pavement friction is a complicated mechanism affected by a variety of factors composed of tire type, pavement surface macrotexture and microtexture, wet and dry conditions, and vehicle speed. Adhesion and hysteresis are primary frictional force components for tire-pavement friction, which are critical to roadway safety. Many numerical approaches have been used to analyze the pavement friction including the finite element method [123–125], discrete element method [126, 127], and

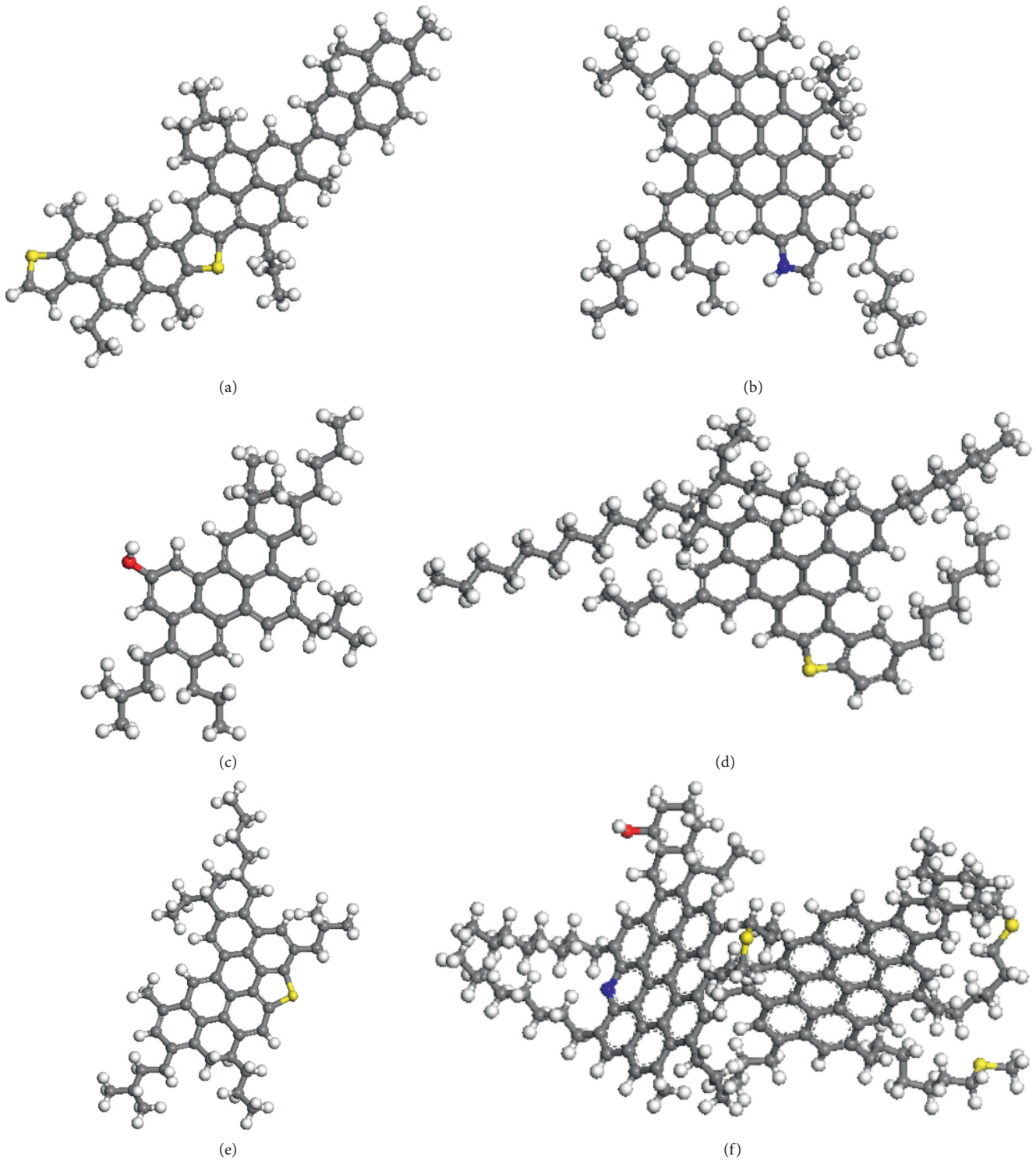


FIGURE 7: Typical molecular structures for asphaltenes [94, 95, 98, 99].

boundary element method [128, 129], at macro-, micro-, and nanoscales. Most of the previous studies on the mechanisms focus on the macro friction behavior based on continuum mechanics. However, the traditional friction analysis cannot reveal the mechanism of tire friction on pavement fully at macro scale.

Recently, some studies have been conducted on the tire friction behavior on pavement at nanoscale [130]. The molecular dynamics method was used to simulate the friction process between the diamond matrix and amorphous carbon probes by Mo et al. [131]. Grierson et al. used the atomic force microscope (AFM) test to study the

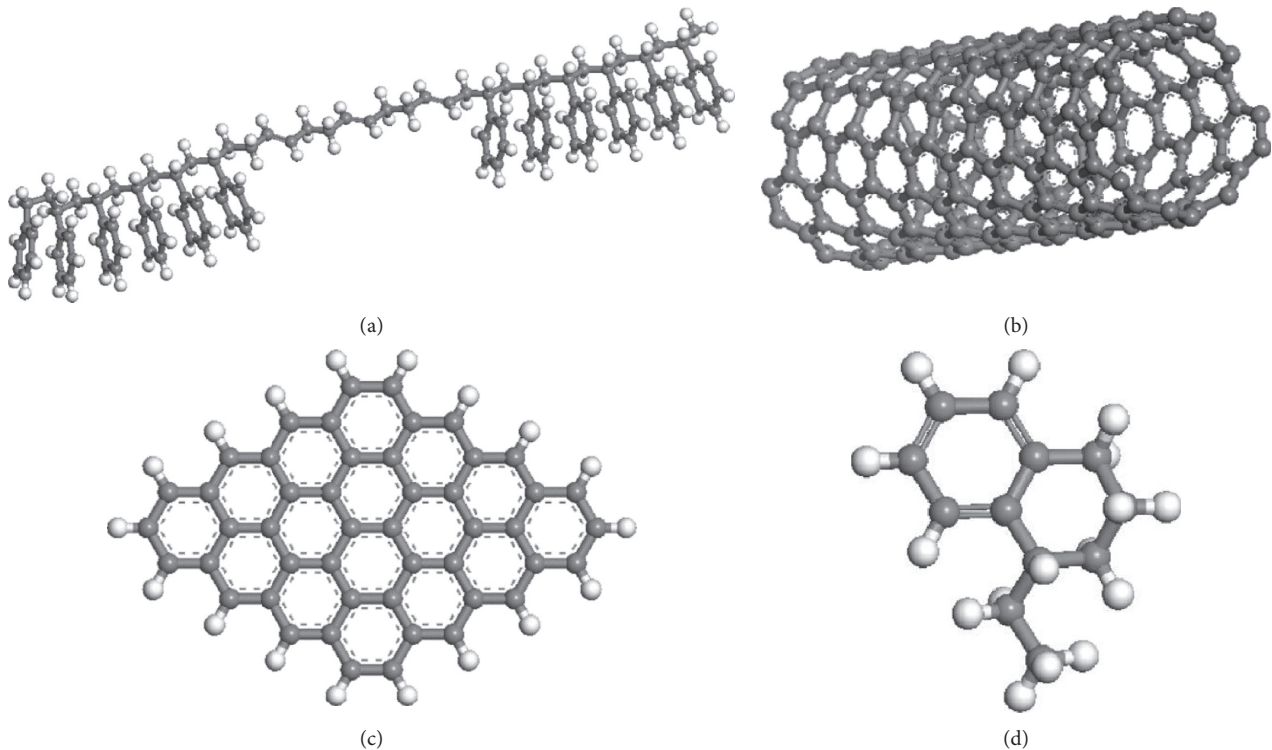


FIGURE 8: Typical molecular structures for modifier [104, 109–111]: (a) SBS, (b) CNT, (c) graphene, and (d) rejuvenator.

adhesion and friction properties at nanoscale [132]. It is found that the friction force has a linear relationship with contact area at the nanoscale. The friction force changes from nonlinear to linear with the decrease of the adhesion between the contacting surfaces [133, 134]. The tribometer, a sophisticated device, is used to clarify the friction coefficient (μT) from the nano-, micro-, and macroscopic texture of a surface [112]. Hou et al. applied the MD simulation to study the microscopic friction of tire on the asphalt pavement, where the MD simulation was conducted under different environments [135]. There are still some MD simulations about the friction proposed for the other material, and these MD simulations are meaningful to review, because these studies can provide some new methodologies for the tire-pavement friction in terms of MD simulation. For example, Shimizu et al. created two molecular models to represent the slider of AFM and specimen, and the friction during the test and the major influencing factors were investigated using MD simulation combining the constitutive model [136].

5. Conclusion

The above review explains that the microscale properties of the asphalt binder significantly affect the macroscale properties with the fast development of technology. The chemical properties of each fraction are therefore studied, and some chemical structures are proposed to study the mechanism of properties of the asphalt binder at molecular scale. Later, the molecular dynamics (MD) simulation was developed because the MD simulation can reflect the

thermodynamics behaviors of asphalt molecules in a dynamic process. MD simulation is a kind of an effective research tool that explores the properties of asphalt binder material from a microscopic perspective.

Using the molecular structure of the asphalt binder and aggregate, the interaction energy between them can be characterized. It is known that the aggregate mineral influences the work of adhesion obviously. It is also employed to explore the influence of water on the adhesion behavior from a micro perspective; some research shows that the interface between the asphalt binder and calcite is susceptible due to moisture damage at small moisture content.

The model of aged the asphalt binder is created by changing the ratio of each fraction, adding some functional groups, or adding some oxygen elements. Then the asphalt binder is studied before and after aging at a molecular scale based on the aged asphalt binder model; meanwhile, the aging mechanism can be also investigated. Based on some microstudy on aging of the asphalt binder, it is seen that there are two reasons for the decrease of molecular diffusion of aged asphalt: on the one hand, the molecular size of asphaltene, resin, and aromatic decreases; on the other hand, free volume space for saturate reduces.

In terms of mechanism of crack, applying some tension on different asphalt binder models, it is found that the atoms distribution at microscale would influence the intrinsic defects of the asphalt binder, and the crack initiation and propagation would be further affected in the asphalt binder.

The modifier is also an important research region of the asphalt MD simulation. The influence law of different modifiers on physical parameters, such as the density and

glass transition temperature of the asphalt binder can be investigated, and the modification characteristics of different modifiers on asphalt performance and their respective modification mechanisms can be further researched. In terms of rejuvenator, its diffusion behavior in the asphalt binders at different aging states can be studied to guide the use of regenerative agents.

As the supercomputer can be used in the future, the model size and the time scale would be increased obviously. In this case, the simulation process will be closer to the macro test, and the simulation result will be closer to the test results.

Disclosure

The authors are solely responsible for the content.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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