Research Article

Effect of Iron Oxide on Self-Healing and Thermal Characteristics of Asphalt Based on Molecular Dynamics Simulation Perspective

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1. Introduction

Many research studies have investigated the self-healing capacity of asphalt. Most were focused on improving its dynamic modulus, flexural stiffness, and viscosity to prolong its service life, as measured by mechanical tests [1–3]. However, those studies did not use image-analysis tools to investigate the healing performance of asphalt binder. In addition, the output of waste metal materials in the construction industry is very large. The waste iron and steel can not only continue to bear loads but also have their own thermal physical properties can be reused. Metal materials can effectively improve the self-healing ability of asphalt, which has been widely verified. Those research studies have mainly focused on the factors influencing the healing ability or on techniques for enhancing the healing effect; less attention has been paid to studying at a microscale level the mechanism of enhancing the healing ability.

To compare the effects of two powders, iron oxide and mineral, on the healing process of asphalt molecules, Fe2O3-asphalt and SiO2-asphalt were constructed by Material Studio software (MS). The mean square displacement, diffusion coefficient, concentration distribution of the asphalt layer, and the thermal conductivity of the two models were analyzed to evaluate the influence of two powders on the diffusion behavior of asphalt molecules on a microlevel. The results show that the effect of Fe2O3 on the diffusion rate of asphalt molecules is greater than that of SiO2 at high temperature, but the effects are similar at low temperature. The diffusion coefficient of the Fe2O3-asphalt model increases faster than that of the SiO2-asphalt model with increasing temperature. Compared with SiO2, Fe2O3 is more conducive to the model’s reaching a state of uniform concentration, which is manifested as the rapid repair of cracks on a macrolevel. The thermal conductivity of the Fe2O3-asphalt model is higher than that of the SiO2-asphalt model.

To investigate the properties of asphalt at a microscale level, asphalt was divided into different components by some chemical composition testing techniques [4–14]. The chemical composition and structure of asphalt can affect its rheological and mechanical capacities [15–18], so it is important to use an accurate molecular model for asphalt. There are many studies exploring asphalt components and systems using molecular models [19]. Corbett et al. separated asphalt into different classes: asphaltenes, polar aromatics, naphthene aromatics, and saturates [20]. A molecular model of asphalt was developed by applying statistical mechanical sampling of the positions, orientations, and configurations in multicomponent systems of relatively few (3–12) molecule types [21–24]. The Hansen solubility parameter was used to understand the components in asphalt models [7]. Researchers have built computational modeling in order to investigate the mechanism of asphalt’s adhesion to a mineral surface [25]. For instance, Fan et al. used molecular...
dynamics (MD) simulation to study the adhesion mechanisms between asphalt and component minerals [26]. Zheng et al. found that the resin and asphaltene, polar molecules of the bitumen component, have good adhesion to the mineral surface [27]. Amirul et al. also pointed that the promotional effect of oxidation on bitumen-silica interactions through computational modeling. Sun et al. investigated the influence of temperature on the self-healing capability of asphalt binder using MD simulation. Analyses of density, relative concentration, and mean square displacement (MSD) were performed to investigate the temperature sensitivity of the self-healing characteristics of asphalt binder [28, 29]. Using small-scale MD simulation, research of the micromechanical healing mechanism of asphalt binder and the influence of crack width on the healing property found that higher temperature would result in higher diffusivity of molecules and thus a higher healing rate [30]. The “compression” of asphalt binder volume and the “stretching” of the asphalt binder molecules were responsible for the disappearance of vacuum microcracks inside the asphalt binder [31]. Using molecular simulation as a research method, Zhou and Li analyzed the feasibility of using the values of the chemical structure indexes H/C and CH2/CH3 as evaluation indexes of asphalt’s self-healing performance. The results showed that the trend was the same as the experiment result [32]. Crack width, temperature, the state of molecular aggregation, and the aggregate have great influence on the self-healing behavior of asphalt binder. In addition, graphene was found to have some positive impact on the self-healing process of asphalt binder [33].

The current studies have been very rich in the exploration of asphalt components and factors affecting asphalt’s self-healing behavior, and a few types of bitumen aggregate have been evaluated under different substrate conditions. However, there is little research on the simulation and analysis of the influence of iron on the healing performance of asphalt binder. A better understanding of metal iron’s influence on asphalt healing behavior can promote the application of scrap metal iron in civil engineering. In addition, iron mineral powder is one of the traditional road construction materials that belong to the pozzolanic activity of materials rich in active SiO2. To explore the effects of the metal iron base and mineral base on the healing behavior of asphalt, Fe2O3 and SiO2 molecular models were selected to compare their difference in heat-conduction performance in asphalt healing.

2. Materials and Methodology

2.1. Construction of Molecular Models of Four Asphalt Components and Asphalt Binder. Based on reference [34], the molecular structure of the asphalt used in this paper adopts a four-stage12-component system, as shown in Table 1. The bitumen model contains three types of asphaltene, five types of resins, two types of saturate, and two types of aromatics. The proportion of each component of 70° virgin asphalt (Table 2) obtained through a four-component test is shown in Table 3.

Under periodic boundary conditions, the asphalt model with an initial density of 0.6 g/cm³ was constructed with the amorphous cell tool. In order to minimize the energy of the asphalt model and eliminate adverse contact, the system needs to be geometrically optimized. At 298.15 K, an isothermal-isobaric (NPT) ensemble was applied at a pressure of 1 atm to run 100 ps at a time step of 1 fs to obtain a sufficiently balanced model of the system. Then, in order to obtain a stable molecular model, the canonical ensemble (NVT) was continued, and the time step remained 1 fs after another 100 ps run. In the two dynamic operations, the truncation distance was 15.5 Å (1 Å = 0.1 ns), the temperature control mode was velocity scale, and the temperature difference was 10 K to control the temperature of the system. Figure 1 shows a pure asphalt model with the lowest energy.

2.2. Molecular Dynamics Model Verification. To ensure that the asphalt molecular model can obtain reliable data results after dynamic calculation, the density of a single asphalt model was calculated according to the literature [35]. Operating in the Forcite-dynamic module, whose force field is COMPASS at six temperatures (298.15 K, 313.15 K, 333.15 K, 353.15 K, 373.15 K, and 393.15 K), the dynamic calculations were carried out under the conditions of 373.15 K and 393.15 K, NPT ensemble, 1 atm pressure, simulation time of 200 ps (1 ps = 10^-12 s), and Nose–Hoover as the temperature-control method, based on the theory study in reference [36]. The density of the pure asphalt model changed with simulation time, as shown in Figure 2. The results in Figure 2 show that the density of the asphalt molecular model increases with the increase in simulation time. Then, after 50 ps, the density tends to stabilize. In addition, the simulation results also show that the density of the model decreases with increasing temperature; this is consistent with the results obtained in reference [36], which proves that the established asphalt model is reliable.

2.3. Construction of the Crystal Structure of Minerals. Fe2O3 was used as a representative of iron oxide metal, and the model of metal-iron-mineral-asphalt was established. SiO2 occupies a large proportion in conventional aggregates; it can usually account for more than 40% of the total composition of aggregates. (Granite is a widely used aggregate in road construction, and the proportion of SiO2 is as high as 72% in granite). Therefore, to establish an interface model between different minerals and asphalt, SiO2 was used to represent common minerals, so that the structural behavior of the mineral-asphalt interface can be studied at a microscopic scale.

The lattice parameters of Fe2O3 and SiO2 cells are shown in Table 4. To establish two representative oxide substrates, these are the operation steps:

(1) Import Fe2O3 and SiO2 cells (Figure 3) into Materials Studio from CRYSTAL Data Center (CCDC).

(2) Set the structural surface. According to reference [37], the crystal structures of Fe2O3 and SiO2 are
Table 1: The 12 components of bitumen grade 4 (carbon is grey, sulfur is yellow, hydrogen is white, and oxygen is red).

<table>
<thead>
<tr>
<th>Components</th>
<th>Molecular models</th>
</tr>
</thead>
<tbody>
<tr>
<td>Asphaltene</td>
<td>![Asphaltene Molecular Model]</td>
</tr>
<tr>
<td>Resin</td>
<td>![Resin Molecular Model]</td>
</tr>
<tr>
<td>Saturate</td>
<td>![Saturate Molecular Model]</td>
</tr>
<tr>
<td>Aromatic</td>
<td>![Aromatic Molecular Model]</td>
</tr>
</tbody>
</table>

Table 2: Technical parameters of 70# base asphalt.

<table>
<thead>
<tr>
<th>Technical parameters</th>
<th>Technical standards</th>
<th>Testing results</th>
</tr>
</thead>
<tbody>
<tr>
<td>Penetration (25°C, 5 s, 100 g)/0.1 mm</td>
<td>60~80</td>
<td>62</td>
</tr>
<tr>
<td>Soft point (°C)</td>
<td>≥46</td>
<td>48.5</td>
</tr>
<tr>
<td>Ductility (15°C)/cm</td>
<td>≥100</td>
<td>&gt;100</td>
</tr>
</tbody>
</table>

Table 3: Ratios of asphalt four-component test.

<table>
<thead>
<tr>
<th>Components</th>
<th>Units</th>
<th>Testing ratios</th>
<th>Simulation ratios</th>
<th>Methods</th>
</tr>
</thead>
<tbody>
<tr>
<td>Asphaltene</td>
<td>%</td>
<td>17.55</td>
<td>17.502</td>
<td>NB/SH/T 0509-2010</td>
</tr>
<tr>
<td>Resin</td>
<td>%</td>
<td>48.58</td>
<td>47.442</td>
<td>NB/SH/T 0509-2010</td>
</tr>
<tr>
<td>Saturate</td>
<td>%</td>
<td>7.73</td>
<td>8.378</td>
<td>NB/SH/T 0509-2010</td>
</tr>
<tr>
<td>Aromatic</td>
<td>%</td>
<td>26.14</td>
<td>26.672</td>
<td>NB/SH/T 0509-2010</td>
</tr>
</tbody>
</table>
shear along the normal direction of [0, 0, 1]. Since the no-bond cut-off value is set to 9.5a in the force field setting, the surface depth must be greater than 9.5a. In this paper, the cut-off distance is set to 15.5a.

(3) Increase surface area. During the process of layer building, the model will stretch or compress if the volume parameter is different, this leads to distortion of the final calculation. Therefore, according to the volume parameters of the asphalt molecular model established above, when increasing the crystal surface volume, the size of crystal base model should be as close as possible to that of the asphalt model, and the size of the two substrates should be as similar as possible. Building vacuum slab and supercell were used to increase the surface area of the two sections by repeating in the X and Y directions, and then the period was changed from 2 to 3 dimensions.

(4) Use geometric optimization to obtain an optimal structure. Finally, the mineral-crystal cell model for layer construction was obtained, as shown in Figure 4. Because of silica’s strong surface reactivity, it is easily hydroxylated in the presence of water [29]. When establishing the crystal model of SiO₂ based on reference [28], a 4.5OH group/Nm² silicon dioxide film representing complete hydration was added. Therefore, to increase the reliability of calculation results in the system, the hydrogenation operation was carried out after the crystal model of SiO₂ was established (Figure 5).

2.4. Construction of Mineral-Asphalt Molecular Model with a Crack. Models of asphalt with different substrates were built using the Build layers tool, and 10 Å vacuum was set as a crack width in the asphalt. The selection model size was matched according to average size. To ensure that the entire system was in a state of energy minimization, geometric optimization was carried out on the entire system again, and the number of iterations was 10000. The optimized mineral-asphalt model is shown in Figure 6.

2.5. Molecular Dynamics Simulation

2.5.1. Healing Behavior. In reference to the literature [28], the Forcite module was used for dynamic simulation calculations. Since asphalt is a kind of polymer material, COMPASS was used, and the dynamic simulation calculation was carried out under the constant temperature and constant volume NVT ensemble. First, it was run for 500ps at a time step of 0.1fs. The atom-based summation was suitable for van der Waals interaction, and the truncation radius was set to 15.5 Å to obtain accurate data. Then, the time step was changed to 1 fs and it was run for 500ps with the truncation radius unchanged. Finally, the same dynamic calculation was performed for two models under different temperature conditions. In the simulation calculation process, the control method selection of temperature is particularly important. To ensure the accuracy of the temperature, the Velocity Scale and Nose–Hoover temperature control methods were adopted successively, and the temperature difference was set at 5 K.

2.5.2. Diffusion Coefficient. The diffusion coefficient was used to characterize the diffusion property of asphalt molecule on the surface of two minerals. The law of

<table>
<thead>
<tr>
<th>Mineral oxides</th>
<th>Edge length (Å)</th>
<th>Crossing angle (°)</th>
<th>a</th>
<th>b</th>
<th>c</th>
<th>α</th>
<th>β</th>
<th>γ</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe₂O₃</td>
<td>5.035</td>
<td>5.035</td>
<td>13.720</td>
<td>90</td>
<td>90</td>
<td>120</td>
<td></td>
<td></td>
</tr>
<tr>
<td>SiO₂</td>
<td>4.913</td>
<td>4.913</td>
<td>5.4052</td>
<td>90</td>
<td>90</td>
<td>120</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Figure 1: Molecular model of asphalt.

Figure 2: Molecular density values at different temperatures.
molecular diffusion can indirectly indicate the process of damage healing. This is because the healing behavior of asphalt can be interpreted as the process of asphalt molecules gradually moving to the damage site, and finally, the repair of damage cracks can be completed to achieve the healing effect. The diffusion coefficient is usually given in the
Einstein expression [38], as shown in the following equation. The limiting slope of the MSD curve as a function of time can be used to evaluate the diffusion coefficient of particles. Usually, the diffusion coefficient can be simplified to this [39]:

$$D = \frac{1}{6} \lim_{t \to \infty} \frac{d}{dt} \sum_{i=1}^{N} \left\{ [r_i(t) - r_i(0)]^2 \right\},$$  \hspace{1cm} (1)

By averaging over all atoms, the MSD would have a linear dependence on time. Thus, the diffusion coefficient, \(D\), could be derived from the slope of the MSD–time relationship, as in the following equation. The unit of \(D\) is \(\AA^2/\text{ps}\).

$$D = \frac{1}{6} \lim_{t \to \infty} \frac{d}{dt} \text{MSD} = \frac{a}{6},$$  \hspace{1cm} (2)

where \(a\) is the slope of the straight line fitted by MSD versus simulation time. The unit of \(a\) is \(\AA^2/\text{ps} \) or \(10^{-8} \text{ m}^2\text{s}^{-1}\). The slope of curves can be obtained by fitting the relationship between MSD and simulation time. The diffusion coefficients of asphalt fractions at different temperatures can be calculated according to equation (2).

2.5.3. Time Series Methodology. The time series method is a method that can predict the law of sequence development. It is also called the simple denotation method. It is a statistical method that can predict the future development trend of data based on the law of past data. Time series refers to a series of data arranged in chronological order. Time series analysis is a mathematical process used to analyze dynamic data. It is based on stochastic process theory and statistical methods to get the statistical law of the research object. Traditional statistical analysis is based on independent data series, while time series analysis focuses on the interdependent relationship between the data of the research object. General statistical analysis also includes autocorrelation coefficient (ACF) and partial autocorrelation coefficient (PACF). Based on time series theory [40], John’s Macintosh Product (JMP) software was used to obtain partial autocorrelation coefficients of asphalt molecular models in the OX and OY directions at 298.15 K temperature, to judge the stability of relative concentration data.

2.5.4. Calculation Methodology of Thermal Conductivity. If the density of the model system is not uniform during the calculation process of thermal conductivity, it would affect the thermal conductivity calculation, leading to a result that does not conform to the actual situation. Since the existence of voids would reduce the transmission rate of heat flow between divided layers, the goal was to obtain a model with uniform density and as few voids as possible. Therefore, the model, as shown in Figure 7 was adopted, and the dynamic calculation was carried out after the modeling was completed. COMPASS was used for the force field, the temperature was set at 298.15 K, and the time step was 1 fs. The calculation time was 1000 ps, and then the thermal conductivity was calculated.

First, the force field setting of atoms in the model should be changed to universal, and the current charge should be used by default before the calculation of thermal conductivity. Then, the script of thermal conductivity should be run. To reduce the time cost of calculation and ensure the accuracy of calculation results, the number of layers along the Z-axis was set at 40 in this section. To obtain the influence of two different base models on the temperature distribution and transfer of the asphalt model, the temperature field results were calculated. Set the time step to 1 fs and the number of steps to 250 fs. The temperature control method was Berender, and the temperature attenuation constant was set to 0.1.

3. Results and Analyses

3.1. Mean Square Displacement. Mean square displacement (MSD) can be used to reflect the change of molecular displacement with simulated time so that the law of molecular diffusion can be studied. And the damage-healing behavior of asphalt material is a macroscopic manifestation of molecular motion, so MSD can indirectly reflect the healing behavior of asphalt.

Figure 8 shows the calculated results of MSD from Fe2O3-asphalt and SiO2-asphalt models at different temperatures. For both models, MSD increased with the increase of simulation time, which corresponds to the fact that things always develop in the direction of entropy increase. In addition, the slope of the MSD curves of the two models increased with the increase in temperature, which indicates that a higher temperature leads to a faster diffusion rate of molecules.

3.2. Molecular Diffusion Coefficients. The diffusion coefficients obtained by formula (2) are shown in Tables 5 and 6. The diffusion coefficients (\(D\)) of the Fe2O3-asphalt model were both greater than those of the SiO2-asphalt model at a temperature which was greater than 333.15 K, and the growth rate of the \(D\) value of the Fe2O3-asphalt model was greater with the increase of temperature. When the temperature was 298.15 K and 313.15 K, MSD curve of two models were close, which means that the diffusion behavior of asphalt molecule is not obvious in two models, that is, the repair ability of asphalt molecule is weak at these two temperatures [29]. However, when the temperature was lower than 333.15 K, the diffusion coefficient of the Fe2O3-asphalt and SiO2-asphalt model were unstable, which may be caused by the relatively low temperature, the difference of influence of Fe2O3 and SiO2 on the diffusion behavior of asphalt was not very large. In addition, combined with the conclusions obtained from reference [35], it can also be shown that under a certain condition, Fe2O3 has a stronger promoting effect on the diffusion behavior of asphalt, and this effect would be more significant at a higher temperature, indicating a higher rate of completion of the healing process.

By fitting the relationship between diffusion coefficient and temperature with an exponential function, the results were obtained, as shown in Figure 9. It can be seen that the diffusion coefficient of the Fe2O3-asphalt model grew faster.
**Figure 7:** Thermal conductivity calculation model.

**Figure 8:** Mean square displacement of the Fe$_2$O$_3$-asphalt model and the SiO$_2$-asphalt model at different simulated temperatures.

**Table 5:** Fitting results of diffusivity of Fe$_2$O$_3$-asphalt model at different temperatures.

<table>
<thead>
<tr>
<th>Temperature (K)</th>
<th>Fitting equation of MSD curve</th>
<th>Diffusion coefficient ($D/10^{-10}$ m$^2$s$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>298.15 K</td>
<td>$y = 0.2753x + 8.6126$, $R^2 = 0.9949$</td>
<td>4.59</td>
</tr>
<tr>
<td>313.15 K</td>
<td>$y = 0.2305x + 8.5681$, $R^2 = 0.9984$</td>
<td>3.84</td>
</tr>
<tr>
<td>333.15 K</td>
<td>$y = 0.5102x + 12.883$, $R^2 = 0.9982$</td>
<td>8.5</td>
</tr>
<tr>
<td>353.15 K</td>
<td>$y = 0.6722x + 15.726$, $R^2 = 0.9978$</td>
<td>11.2</td>
</tr>
<tr>
<td>373.15 K</td>
<td>$y = 0.9828x + 17.885$, $R^2 = 0.9998$</td>
<td>16.38</td>
</tr>
<tr>
<td>393.15 K</td>
<td>$y = 1.6583x + 28.153$, $R^2 = 0.9979$</td>
<td>27.64</td>
</tr>
</tbody>
</table>

**Table 6:** Fitting results of diffusion coefficients of SiO$_2$-asphalt model at different temperatures.

<table>
<thead>
<tr>
<th>Temperatures (K)</th>
<th>Fitting equation of MSD curve</th>
<th>Diffusion coefficient ($D/10^{-10}$ m$^2$s$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>298.15 K</td>
<td>$y = 0.2309x + 8.5098$, $R^2 = 0.9913$</td>
<td>3.85</td>
</tr>
<tr>
<td>313.15 K</td>
<td>$y = 0.2575x + 9.8902$, $R^2 = 0.9951$</td>
<td>4.29</td>
</tr>
<tr>
<td>333.15 K</td>
<td>$y = 0.654x + 11.53$, $R^2 = 0.9997$</td>
<td>10.9</td>
</tr>
<tr>
<td>353.15 K</td>
<td>$y = 0.6091x + 14.41$, $R^2 = 0.9943$</td>
<td>10.15</td>
</tr>
<tr>
<td>373.15 K</td>
<td>$y = 0.6961x + 18.143$, $R^2 = 0.9987$</td>
<td>11.6</td>
</tr>
<tr>
<td>393.15 K</td>
<td>$y = 1.5049x + 27.552$, $R^2 = 0.9845$</td>
<td>25.08</td>
</tr>
</tbody>
</table>
than that of the SiO2-asphalt model with the increase of temperature, which indicates that Fe2O3 enhances the sensitivity of asphalt to temperature and increases the diffusion rate of molecules, thus indirectly improving the damage healing rate and healing ability of asphalt.

### 3.3. Relative Concentration in OX, OY, and OZ Directions

#### 3.3.1. Relative Concentrations in OX and OY Directions

The distribution of atomic concentration in the asphalt molecule can be used to reflect its motion characteristics and rules. Therefore, the concentration distribution can be obtained by calculating the atomic density of periodic structures with cracks parallel to each coordinate axis, so as to evaluate the motion behavior of the asphalt molecule, and then evaluate its damage healing effect and rate.

After dynamic simulation, the relative concentrations in the OX, OY, and OZ directions were obtained, as shown in Figures 10 and 11. The figures show that the relative concentrations of the asphalt model in the OX and OY directions were almost constant. This was consistent with the total concentration, and the concentration distribution was more uniform with a higher temperature. It can be concluded that in the process of crack repair, in both the Fe2O3-asphalt model and the SiO2-asphalt model, the motion of asphalt in the direction of OX and OY tended to be stable. This is the same as the motion of atoms in OX and OY directions under the pure asphalt model [29]. It showed that the healing behavior in the OX and OY directions was not obvious, since there was no damage crack, the asphalt molecules were in a relatively balanced state, and their motion behavior was relatively gentle.

#### 3.3.2. Partial Autocorrelation Coefficient

The change in relative concentration can indicate that the asphalt molecules move during the process of asphalt healing, thus showing the healing behavior. When the asphalt concentration around the crack increases, it indicates that the crack is being repaired.

It can be seen from Figures 12 and 13 that the development trend of partial autocorrelation coefficient of each different lag number was 0, which indicates that the time series data studied was stable. In other words, the relative concentrations of the asphalt model in the OX and OY directions of the two models were consistent with the total concentration, and remained almost unchanged after the dynamic simulation was started. Therefore, it can be concluded that the motion of asphalt molecules in these two directions tends to be stable at a density of 1.0.

#### 3.3.3. Relative Concentrations on OZ Direction

Through the calculation on the direction of (0, 0, 1) to estimate the relative concentration of asphalt molecular aggregation distribution in the OZ direction, Figure 14 shows the asphalt molecular distribution in the OZ direction. It can be seen from the diagram, for the initial model, the vast majority of asphalt molecules were distributed at both ends of the model, and the atomic concentration at the cracked part was 0. After a dynamic calculation at different temperatures, the atomic concentration of the cracked part began to increase. This was due to the atoms in the two layers of asphalt molecules being close to each other to repair the cracked area, so the relative concentration gradually increased. In addition, at different ambient temperatures, with the increase in temperature, the atomic concentration of the cracked part increased gradually, and the concentration value after healing was progressively closer to 1.0 g/cm³.

However, it is not enough to analyze only the concentration distribution of asphalt in the composite model; the numerical difference of its relative concentration was not very significant, which makes it difficult to distinguish the influence of Fe2O3 and SiO2 on the motion of asphalt molecules. Therefore, the standard deviation of relative concentration in the asphalt molecular model was calculated at different temperatures to obtain the influence of the
two different substrates on the uniformity of the asphalt concentration distribution in the models. The results are shown in Figure 15. It can be seen that with an increase in temperature, the standard deviation became progressively smaller, indicating that the distribution of asphalt components was more uniform. Compared with the SiO2-asphalt model, the standard deviation of the relative concentration in the Fe2O3-asphalt model was smaller. It can be concluded that the distribution of the asphalt components in the Fe2O3-asphalt model was more uniform. At higher temperatures, asphalt components in the Fe2O3-asphalt model could reach the equilibrium state more rapidly and complete the repair of cracks. When the temperature was lower, the composition distribution uniformity of the two models was relatively close. That is because the flow performance of asphalt at a lower temperature is poor, and it is not enough to complete the crack-repair process; therefore, the overall standard deviation value is larger, and the relative concentration of the two models became more similar.
different bases would not produce a significant effect on the distribution of asphalt components.

3.4. Thermal Conductivity. The thermal conductivity of the Fe$_2$O$_3$-asphalt model and the SiO$_2$-asphalt model obtained by dynamic calculation is shown in Table 7. The results were

![Figure 12: Partial autocorrelation coefficients of Fe$_2$O$_3$-asphalt model (a) and SiO$_2$-asphalt model (b) in the OX direction.](image)
Figure 13: Partial autocorrelation coefficients of Fe₂O₃-asphalt model (a) and SiO₂-asphalt model (b) in the OY direction.

Figure 14: Relative concentration distributions of Fe₂O₃-asphalt (a) and SiO₂-asphalt (b) in the OZ direction.
0.3873 W/m/K for the Fe$_2$O$_3$-asphalt model and 0.1969 W/m/K for the SiO$_2$-asphalt model. This indicates that the Fe$_2$O$_3$-asphalt model has a higher heat-flow exchange rate under the same temperature condition, so it can raise the temperature of the model at a faster rate. This characteristic was conducive to the asphalt binder starting the healing behavior earlier and thereby improving its healing ability.

4. Conclusions

The Fe$_2$O$_3$-asphalt model and a SiO$_2$-asphalt model were established, and dynamic simulations and thermodynamic calculations were carried out under different temperature conditions. The mean square displacement, diffusion coefficient, concentration distribution of the asphalt layer, and the thermal conductivity of the two models were analyzed. Maybe the influence of other metal oxide on the healing property of asphalt on microlevel and macrolevel could also be researched in the future. It would enrich the research of asphalt area. The main findings of this study can be drawn as follows:

(1) A higher temperature leads to a larger diffusion rate of molecules. At different temperatures, the mean square displacement (MSD) of Fe$_2$O$_3$-asphalt and SiO$_2$-asphalt model increased with the increase of simulation time. The slope of MSD curve increased with an increase in temperature.

(2) Fe$_2$O$_3$ has a better effect on the diffusion rate of asphalt molecules than SiO$_2$ at a higher temperature, but it is similar at a lower temperature. At a temperature greater than 333.15 K, the diffusivity of the Fe$_2$O$_3$-asphalt model was greater than the diffusivity of the SiO$_2$-asphalt model.

(3) Fe$_2$O$_3$ enhances the sensitivity of asphalt materials to temperature and increases the diffusion rate of molecules. The diffusion coefficient of the Fe$_2$O$_3$-asphalt model increased faster than that of the SiO$_2$-asphalt model with increasing temperature. And the exponential parameter of the Fe$_2$O$_3$-asphalt model is larger than that of the SiO$_2$-asphalt model.

(4) Under different temperature conditions, the standard deviation of the relative concentration of the asphalt molecular in Fe$_2$O$_3$-asphalt model was smaller.

(5) The thermal conductivity of Fe$_2$O$_3$-asphalt model is higher than that of SiO$_2$-asphalt model at 298.15 K. This helps to get to the healing temperature as soon as possible, then to bring forward the start time of fracture healing and indirectly improve the self-healing ability of asphalt.

Data Availability

The data used to support the findings of this study are available from the corresponding author upon request.

Conflicts of Interest

The authors declare that they have no conflicts of interest.
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