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Research on the Adhesion and Self-healing Properties of Bio-asphalt Based on Molecular Simulation

Yuan Fu [1], Meng Wu [2], Tianqing Hei [2], Zezhen Dong [2], Jianying Hu [2], Weiguang Zhang [2*]

[1] Highway Administration of Shanxi Province, 030006, Taiyuan, China

[2] School of Transportation, Southeast University, 211189, Nanjing, China

(wgzhang@seu.edu.cn)

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ABSTRACT

At present, the extraction of new bio-asphalt materials from renewable energy sources has become the focus of research in the field of pavement engineering. Bio-asphalt has the characteristics of wide source, low cost, green, pollution-free and is also renewable. With the expansion of the application range of bio-asphalt, its adhesion to aggregates and the healing properties after damage have received extensive attention. In this paper, the bio-asphalt-aggregate adhesion and healing behaviors were evaluated and compared using molecular dynamics approaches. Firstly, the molecular models of vegetable oil bio-asphalt and waste edible oil were established, and the two bio-asphalt molecular models were verified according to the physical quantities such as density, viscosity, cohesive energy density (CED), glass transition temperature and solubility parameter. Then, the bio-asphalt-aggregates interlayer model was established, and the adhesion energy and the energy ratio (ER) value under water conditions were calculated and analyzed using energy theory. A bio-asphalt self-healing model was established, and concentration distribution and diffusion analysis were performed. The results show that the viscosity of bio-asphalt is significantly lower than that of base asphalt, and the shear resistance becomes lower at high temperature. In terms of adhesion, bio-asphalt has better temperature sensitivity. The two bio-asphalts have better adhesion than base asphalt and silica at different temperatures, especially at high temperature (65 °C). There was no significant difference between the adhesion energy of the two bio-asphalts. Bio-asphalt is more affected by water intrusion, and its ability to resist water damage is significantly weaker than that of base asphalt. The NPT density-time curve, concentration distribution and MSD calculation results all showed that the self-healing performance of bio-asphalt was better than that of base asphalt, while the two bio-asphalts showed little difference in healing performance.

Keywords:

Bio-asphalt, interfacial adhesion, Self-healing performance, Molecular simulation.