Chapter 13

Molecular Dynamics Simulation of Asphal tic Material: Molecular Dynamics Simulations of Oxidative Aging of Asphalt Molecules under Stress and Moisture

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ABSTRACT

An attempt is made to understand the chemical composition, oxidation mechanisms, and property changes of asphalt binders before and after oxidative aging using molecular dynamics (MD) simulations. Unoxidized and oxidized asphalts are subjected to different compressive and tensile stress rates, and moisture contents at room temperature. Results show that density, energy, and viscosity of the oxidized asphalt are higher than the unoxidized asphalt, indicating hardening and rheological property changes of asphalt after oxidation. Both the unoxidized and oxidized asphalts deform more and fail faster with an increase in stress rates, especially under tensile stress. The oxidized asphalt is stronger than the unoxidized asphalt under mechanical stress. Moisture inclusion affects viscosity more by decreasing the viscosity of the oxidized asphalt faster compared to the unoxidized asphalt. The viscosity of the oxidized asphalt is lower than that of the unoxidized asphalt above 5% moisture inclusion. This indicates that oxidized asphalt pavement might be exposed to more moisture-induced damage.

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INTRODUCTION

Asphalt, also known as bitumen, is a petroleum product obtained by the distillation of crude oil and is widely used as a binder for roadway construction in the United States. Asphalt is a complex mixture of organic molecules that vary widely in composition from nonpolar saturated hydrocarbons to highly polar and highly condensed aromatic ring systems (Petersen, 1984). The physical properties of asphalt depend on the underlying chemical composition and chemical properties of the composition (Greenfield, 2011). During service life, the chemical composition or molecular structures of asphalt binder changes due to oxidative aging, variable temperature, loads, and field moisture. These changes often adversely affect the performance and/or durability of asphalt pavement.

In reality, there are two major chemical factors affecting asphalt durability: the compatibility of the interacting components and the resistance of the molecules’ chemical composition to change when reacting with atmospheric oxygen respectively (Petersen, 1984). The latter is also called oxidative aging that leads to hardening of the asphalt, which further contributes significantly to asphalt pavement embrittlement and eventually results in excessive pavement cracking (Petersen, 2009).

Moreover, another major concern of asphalt pavement is moisture damage (Ma, Huang, Mahmoud, & Garibaldy, 2011), which is caused by water penetrating into the asphalt-aggregate system and results in rheological property change of the asphalt binder that shortens the binder’s service life and debonds the asphalt from aggregates to accelerate pavement distresses (Chindaprasirt, Hatanaka, Mishima, Yuasa, & Chareerat, 2009). Thus, this chapter is aimed to understand the oxidative aging and moisture damage mechanisms, the chemical composition and property changes of asphalt after oxidative aging, and the combination effects of oxidative aging and moisture damage on asphalt. Molecular dynamics simulation (MD) method is employed to understand these complex properties and mechanisms.

BACKGROUND

MD simulation computes, using a computer, the motion of a series of atoms, their co-ordinates in three-dimensional space, and their connectivity in a system as a function of time. It solves the classical equations of motion of \( N \) atoms interacting via a potential \( U \), the sum of the pair potential of all the atoms. In Cartesian coordinates, the equation of motion is simply Newton’s second law of motion:

\[
a_i(t) = \frac{dv_i(t)}{dt} = \frac{d^2r_i(t)}{dt^2} = \frac{F_i}{m_i}
\]

(1)

where, \( r_i \) is the position of an atom \( i \), \( m_i \) is the mass of the atom, \( a_i \) is the resulting acceleration of the atom, \( v_i \) is the resulting velocity of the atom, and \( t \) is time. The force \( F_i \) acting on the atom is defined as the negative gradient of the potential \( U \):

\[
F_i = -\frac{dU_i(r)}{dr_i}
\]

(2)