Chapter XVI
Computer Simulation of Particle Packing in Bituminous Concrete

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ABSTRACT

Although computer simulation methods have been used extensively in modeling the microstructure of Portland cement concrete, their application for studying asphalt concrete is relatively new. In this chapter, the nature and distribution of inter-particle contacts in computer-simulated compacts with a wide particle size range such as those found in asphalt pavements are discussed. The aggregates were modeled as hard spheres and some typical aggregate gradations used in AC were packed using a computer program. The application of particle packing simulation concepts discussed in this chapter to the study of aggregate structure in asphalt pavements, in conjunction with the recent advances in nondestructive imaging techniques and DEM simulations have tremendous potential to help us to develop a deeper understanding of the aggregate structure in asphalt concrete, develop and optimize the various parameters that describe the aggregate structure and relate them to the performance of pavements in a scientific way.

INTRODUCTION

Asphalt concrete (AC) or bituminous concrete is a composite material consisting of mineral aggregates, asphalt binder and air in a ratio 80:10:10 (by volume), respectively. Currently, choosing the gradation to construct the pavement is based on experience and consensus. It will be of benefit to the pavement community to develop computer modeling techniques to better understand the aggregate structure and its dependence on various factors such as surface roughness, angularity, etc. of the

aggregates and various properties of the binder. The ultimate goal is to model the microstructure of AC using volumetrics and particle packing concepts to predict the volumetric properties for given aggregate properties and gradation.

The modeling work can begin by simulating the packing of spherical /ellipsoid particles having a specified gradation, then add other factors such as surface roughness, presence of asphalt binder and aggregate angularity. The model is expected to calculate characteristics of the compacted asphalt mixture such as bulk density, voids content, void distribution, average coordination number of each particle, etc., and yield information useful to mixture design and particulate mechanics modeling of asphalt concrete.

Particle packing has both theoretical and practical importance in many areas of science and engineering. Computer simulation of particle packing is becoming increasingly attractive with the rapid increase in computing power. Particle packing simulations have been widely applied to mono-size particles (Visher and Bolsterli, 1972; Jullien and Meakin, 1987), particles with a slight spread in sizes (Soppe, 1990), and log-normal distributions spanning as much as 1.5 decades in sizes (Powell, 1980).

In some industries, it is necessary to deal with wide particle size distributions. For instance, the aggregates used in asphalt pavements typically have a 19 mm maximum size and about 5% of the particles (by weight) finer than 75 μm—a span of two and a half decades. In such cases, in order to have a representative number of large particles (25-mm particles), tens of millions of small particles have to be considered. Such simulations present significant challenges in terms of both computing requirements and algorithms to handle particles two orders of magnitude next to one another.

The effect of the size distributions on packing characteristics of the particle have been primarily studied through physical experiments (Sohn and Moreland, 1968; Dexter and Tanner, 1972) and through computer simulations (Nolan and Kavanagh, 1992). In areas such as ceramics and powder metallurgy, a particle system (e.g., powder) with a spread of particle sizes is closely approximated to a known size distribution and is studied by computer simulated packing of spheres. These studies have typically used log-normal or Gaussian particle size distributions with systematic variation of the standard deviation (or range of particle sizes). In these studies, it was found that the packing fraction increased when the standard deviation of the distribution increased.

In many of these studies, a rather narrow size range was considered. Nolan and Kavanagh (1992) used a particle size range of 0-20, while Powell (1980) used sizes from 0 to 1.0, and Bierwagen and Saunders (1974) used particles of sizes from 0.1 to 10, a 2-decade range. In the systems that were of primary interest to the authors, asphalt concrete, this was not an adequate range of distribution of sizes.

The Discrete Element Method (DEM) (Cundall and Strack, 1979) has been used for modeling granular systems. In order to extend the DEM techniques to real aggregates, one major step involves using a range of particle sizes. Zhong et al. (2000) developed methods to use this technique for accommodating particles with sizes spanning two decades. The determination of the initial structure of the granular assembly is an important input to this modeling. The typical technique to obtain this starting assembly is particle packing simulations. Although computer simulation methods have been used extensively in modeling the microstructure of Portland cement concrete (Bentz, 1997), their application for studying asphalt concrete is relatively new. In this chapter, the nature and distribution of inter-particle contacts in computer-simulated compacts with a wide particle size range such as those found in asphalt pavements are discussed. First, it is important to understand how stress is transmitted in asphalt concrete under traffic loading.