Exhibit D

Research Project Requirement Template

A Screening Tool for Assessment of Moisture-Induced Damage of Asphalt Mixes Containing RAP Based on Molecular Dynamics Simulation

Recipient/Grant (Contract) Number: 69A3552348306 (CY1-LTU-02)

Center Name: Southern Plains Transportation Center (SPTC)

Research Priority: Improving the Durability and Extending the Life of Transportation

Principal Investigator(s): Andrew Peters and Nazimuddin Wasiuddin, Louisiana Tech University

Project Partners: Louisiana Tech University

Research Project Funding: Louisiana Tech University: $48,000 (Federal) and $48,000 (Match)

Proposed Start and End Date: 10/1/2023 to 9/30/2024

Project Description: In this project, the research team seeks to develop a screening tool for the assessment of moisture-induced damage potential of asphalt mixes containing reclaimed asphalt pavement (RAP). Molecular dynamics (MD) simulation, a widely accepted physics-based numerical simulation technique, will be used to examine the compatibility between asphalt binders and aggregates, including RAP. Because rejuvenators are used frequently in asphalt mixes containing RAP, particularly with increased RAP contents, rejuvenators will be included in the MD simulations. Adhesive interactions between asphalt binder and aggregate, in the presence of moisture, will be used as an indicator of compatibility or resistance to moisture-induced damage. Because of the limited budget and timeline, existing asphalt, aggregate, and rejuvenator molecules will be used in the MD simulations. Atomistic molecular dynamics will be used to simulate the binder and aggregate interfaces and determine the interaction energies and adhesive strengths between the binder and the aggregate. Using Bell's model, the pulling velocity $v = v_0 exp(f\, x_b/k_b\, T)$, where x_b is the distance between the equilibrium states and the transition state, and $v_0 = \omega_0 x_b exp\,(-E_b/k_b\, T)$, where f is the external pulling force, x_b is the distance between the equilibrium state and the transition state, k_b is Boltzmann's constant, T is temperature, ω_0 is the natural vibration frequency, and E_b is the adhesion energy, will be quantified. The adhesive strength obtained from the MD simulations will be compared with the direct tensile strength determined in the laboratory using a pneumatic adhesion tensile testing instrument.

The following tasks will be performed to meet the project goals: Task 1: Determine adhesion energy following the procedure described in Gao, P. et al. (Appl. Surf. Sci. 2022, 577, 151930) for standard AAA-1 type binder. Use the asphalt binder model described in Li, D. D. and Greenfield, M. L. (Fuel 2014, 115, 347–356) with SiO2 and CaCO3; Task 2: Determine the adhesion energy as a function of water concentration; Task 3: Calculate the adhesion energy as a function of water concentration for selected additives or rejuvenators; Task 4: Conduct laboratory tests to determine direct tensile strengths; Task 5: Compare adhesion energy obtained from the MD simulations with the direct tensile strength results from Task 4; Task 6: Develop a MS Excel-based interactive spreadsheet based on results from Task 5 that can be used by designers as a tool for evaluating aggregate-binder compatibility in presence of rejuvenators and resistance to moisture-induced damage of asphalt mixes.

US DOT Priorities: This project is related to the USDOT objective of Climate and Sustainability. Characterization of moisture-induced damage and how rejuvenators affect such damage (i.e., level of improvement using rejuvenators) will lead to asphalt mixes with improved resistance to moisture damage and enhance the durability and service life of pavement infrastructure. Consistent with USDOT priorities, this project will provide an opportunity for training graduate students and developing special skills in MD simulations.

Outputs: The following outputs are expected from this project: (1) guidelines for improving the compatibility between binder and aggregate in the presence of water. The MS Excel spreadsheet will be used for this purpose; (2) optimum rejuvenator amount and binder-aggregate compatibility using the results from the MD simulations; (3) a framework for performing future simulations for screening of other binders, rejuvenators, and aggregates.

The research results will be communicated to the broader community via publications in journals with high-impact factors and in conference proceedings. Also, presentations at national conferences such as the Annual Meeting of the Transportation Research Board are expected from this project.

Outcomes/Impacts: Moisture-induced damage is a major contributor to reduced pavement performance and service life. The developed tool will be a valuable resource for the state DOTs, cities, counties, and Tribal transportation agencies for screening asphalt mixes. The research team will work closely with some of these organizations to increase their awareness of the benefits of the screening tool during the design stage.

Final Research Report: