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

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7. Author(s)
Andrew Peters, 0000-0001-5031-2828, https://orcid.org/0000-0001-5031-2828
Nazimuddin Wasiuddin

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9. Performing Organization Name and Address
Program of Civil Engineering
Louisiana Tech University
600 Dan Reneau Dr., Bogard Hall, Room 250
Ruston, LA 71272

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16. Abstract
Moisture-induced damage in asphalt pavements remains a significant challenge for road infrastructure durability. This study investigated the adhesive interactions between asphalt binder and aggregate surfaces, with particular focus on the effects of moisture and polyethylene (PE) modification. Using atomistic molecular dynamics simulations, we quantified the adhesion energy between a model SHRP AAA-1 asphalt binder and SiO2 aggregate surface under various moisture conditions. The simulation methodology was validated by achieving dry adhesion energies (46 mJ/m^2) consistent with experimental measurements. Interestingly, low water concentrations (<0.5 waters per nm^2) initially increased adhesion energy, possibly due to enhanced hydrogen bonding. The addition of PE (2.52 wt%) to the asphalt binder produced two significant effects: it reduced the dry binding energy to 33 mJ/m^2, likely due to PE's non-polar nature, but demonstrated a protective effect against water damage at higher moisture concentrations. While unmodified asphalt showed continuous degradation of adhesion with increasing moisture content, PE-modified binder maintained stable binding energies around 28-29 mJ/m^2 (greater than the 23 mJ/m^2 for unmodified asphalt, which continued to decrease). This stabilization effect appears related to PE's hydrophobic nature, which helps repel water from the asphalt-aggregate interface. These findings suggest PE modification could improve moisture damage resistance in wet conditions, though further investigation of its effects on dry properties is needed.

17. Key Words
Asphalt Binder, Molecular Dynamics, Moisture, Simulation, Adhesion

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FINAL REPORT
SPTC Project Number: CY1-LTU-02

Submitted by
Dr. A. J. Peters (PI)
Dr. N. Wassiudin (Co-PI)
College of Engineering and Science (COES)
Louisiana Tech University

Prepared for
Southern Plains Transportation Center
The University of Oklahoma
Norman, OK

SOUTHERN PLAINS
TRANSPORTATION CENTER

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List of Abbreviations and Acronyms

CHARMM	Chemistry at Harvard Macromolecular Mechanics
DOT	Department of Transportation
FHWA	Federal Highway Administration
MD	Molecular Dynamics
NTL	National Transportation Library
OPLS	Optimized Potential for Liquid Systems
PE	Polyethylene
RAP	Reclaimed Asphalt Pavement
ROSA P	Repository & Open Science Access Portal
SHRP	Strategic Highway Research Program
VMD	Visual Molecular Dynamics

Executive Summary

This research project investigated the adhesion energy between binder and aggregate in asphalt pavements through molecular dynamics simulations. The effect of moisture and polyethylene (PE) modification was considered.

The simulation methodology successfully validated real-world conditions, achieving dry adhesion energies of 46 mJ/m², which aligns with experimental measurements. The study utilized a model SHRP AAA-1 asphalt binder and SiO_2 aggregate surface to represent typical road materials.

An unexpected finding emerged regarding water effects: very low water concentrations (less than 0.5 waters per nm²) initially increased adhesion energy, possibly due to enhanced hydrogen bonding between the binder and aggregate. However, higher water concentrations led to progressive deterioration of adhesion in unmodified asphalt, as expected.

The addition of PE (2.52 wt%) showed mixed effects on performance. Under dry conditions, it reduced binding energy from 46 mJ/m² to 33 mJ/m², attributed to PE's non-polar nature creating weaker interactions with the silica surface. However, in wet conditions, PE demonstrated a protective effect, stabilizing binding energies around 28-29 mJ/m² rather than continuing to decrease like unmodified asphalt. This stabilization effect appears to be related to PE's hydrophobic properties, which help repel water from the asphalt-aggregate interface.

PE modification shows promise for improving moisture damage resistance in wet conditions, though the reduced dry adhesion strength suggests potential trade-offs that need careful consideration.

Several areas warrant further research to build upon these findings. The work should be expanded to include different modifiers, binders, and aggregate types. Additionally, investigating the optimal placement and distribution of PE within the asphalt mixture would be valuable. Longer-term studies using coarse-grained simulations could provide additional insights, especially regarding partitioning at the binder/aggregate interface.

This research provides valuable insights into the molecular-level interactions governing moisture damage in asphalt pavements and offers potential directions for improving road infrastructure durability through PE modification, particularly in moisture-prone conditions. However, careful consideration of the trade-offs between wet and dry performance is necessary before widespread implementation.

Chapter 1. Introduction

The infiltration of moisture into asphalt leads to diminished performance, shortened lifespan, and unforeseen failures, thereby diminishing the performance of road networks. Given that roads are consistently exposed to different types of traffic and weather conditions, the presence of moisture can initiate or worsen both new and preexisting damage. This work performed a fundamental investigation into the adhesive interactions between asphalt binder and aggregate, focusing on the effects of moisture and binder additives, specifically plastic. We used atomistic molecular dynamics to simulate the binder and asphalt interface, measure interaction energies, and measure the adhesive strength between the binder and the aggregate.

Chapter 2. Literature Review

One of the major modes of failure caused by moisture damage is adhesive failure at the binder-aggregate interface. This occurs when the binder dissociates from the aggregate, a process that has been documented since the early 1900s. The difference in polarity between the binder and the aggregate promotes the weakening of the interface, making it especially vulnerable to water intrusion. [1] When the aggregate is dislodged from the binder, a process called stripping, the road prematurely fails, leading to increased maintenance costs and shortened service life. [2]

This type of failure is fundamentally related to the chemical and physical interactions between the binder, aggregate, and water. [3–9] The molecular forces between adhesive and substrate play a crucial role in every adhesive and adherent system, with stronger binder-aggregate interactions reducing the chances of failure.[2] Different binders exhibit varying interactions with water, which affects their susceptibility to moisture damage (Kringos, 2007). [10]

Waste plastics such as polyethylene (PE) are hydrophobic in nature and thus could potentially reduce moisture damage by rejecting water from the binder-aggregate interface. Additionally, because higher viscosity binders are associated with better moisture resistance, [11–14] the viscosity modifying effects of PE could indicate an improvement as well. Recent research has shown that plastic waste modified asphalt can improve pavement performance under certain conditions. [15,16]

The work of adhesion between binder and aggregate is commonly used to evaluate moisture damage resistance. [17] Surface free energy (SFE) is a closely related property that provides fundamental material characterization independent of the mixture. [17,18] While these thermodynamic measurements have proven useful in identifying suitable materials for mitigating moisture damage, some researchers argue that they do not directly quantify engineering strength. .[19,20] As more additives, including waste plastic, are used, the effects of these additives on moisture damage require deeper study.

Simulating the energy of interaction between binder and aggregate has the advantage of direct measurement of the adhesive energy and strength between the binder and the aggregate, as well as easy manipulation of the various relevant parameters. That is, binder components, additives, and moisture content can be easily set to whatever value is desired. Asphalt models have continued to improve in their accuracy such that they are now able to model a wide range of asphalt binders, [21] and are compatible with general forcefields[21,22] allowing the modeling of arbitrary additives in the mixture. This kind of modeling also allows access to atomic-level information, providing insight into the mechanisms behind moisture damage and how it affects the interfacial interactions between binder and aggregate.

Chapter 3. Materials and Methodologies

The binder was modeled using the model developed by Li and Greenfield based on the OPLS (Optimized Potential for Liquid System) forcefield that had been used previously.[23,24] This approach allows a wide array of SHRP (Strategic Highway Research Project) model asphalts to be simulated, and ensured compatibility with OPLS tools to create the various additives required. While many different binders could have been considered, the study was restricted to a model SHRP AAA-1 as a representative binder. Future work could consider the effect of different compositions. LigParGen[25] was used to create the additives. LigParGen simply requires inputting a molecular structure in the form of a SMILES (Simplified Molecular Input Line Entry System) string, so polymers and well-defined additives could be easily modeled. It is also compatible with the aforementioned asphalt binder model. Water was modeled using the TIP3P model.[26,27] While aggregates are formed of a large number of metal oxides, the focus in this short project was on the most common, SiO_2, the main component in granite, a common aggregate [28] The SiO_2 was created using the CHARMM-GUI (Chemistry at Harvard Molecular Mechanics - Graphical User Interface) tool[29] but OPLS parameters were used. Details of the aggregate surface certainly were important but were outside the scope of this project. The study was limited to smooth SiO_2 surfaces.

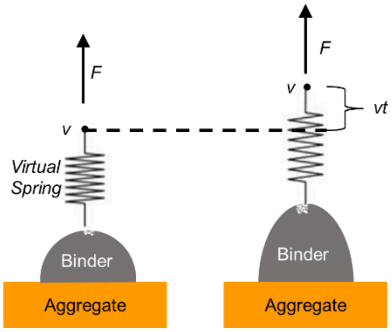

Figure 1. Schematic of simulation to measure binder-aggregate adhesion strength.

Measurement of the adhesion between two materials using molecular dynamics has been well demonstrated in a variety of contexts.[30–32] This project implemented the method described in Reference [30]. The adhesion energy was measured by pulling the asphalt binder off the aggregate using a virtual spring. Using Bell's model,[30,33] the pulling velocity

$$v = v_0 exp(f\, x_b / k_b\, T) \qquad \text{Equation 1}$$

where x_b is the distance between the equilibrium states and the transition state, and

$$v_0 = \omega_0 x_b exp\,(-E_b / k_b\, T) \qquad \text{Equation 2}$$

where ω_0 is the natural vibration frequency, and E_b is the adhesion energy.

The project calculated the adhesion energy as a function of water concentration and validated the results against experimental results under wet and dry conditions with granite. [19,34] Experimental validation came from literature,[35–37] and our own experiments . While granite does not perfectly match the SiO_2 model, the match was sufficient for a reasonable validation. Once validated, water composition was varied. The water was initialized in the empty space between the binder and the SiO_2 and brought to equilibrium. High concentrations of water formed a continuous liquid phase between the binder and the aggregate. In addition to quantifying adhesion, this allowed study of the molecular phenomenon that resulted in adhesive failure.

The effect of waste plastic was investigated. Polyethylene was modeled using LigParGen,[25] however, only small molecular weights (<10kg/mol) were considered as very large molecular weights resulted in very large simulation times and volumes to get accurate data. This was still sufficient to consider the interaction strength between the modified binder and the aggregate, as the main effect of increasing molecular weight, after increasing past some small number, is to increase viscosity and slow dynamics, [38] rather than change the interactions between molecules. Simple monodisperse, low molecular weight models were used. This sped simulation time and provided a good first pass study that could be extended in a future study. Further studies could test a wider range of additives.

Calculation and validation of binding energy and effect of water. A process was created for initiating the asphalt drop above the aggregate surface, and pulling the droplet off the surface at various velocities. The adhesion energy has been calculated for AAA-1 SHRP asphalt with SiO_2 at values similar to those found in literature (See Results and Discussion for a more thorough explanation).

Water was incorporated into simulations and calculations. In addition, multiple runs were used to estimate error. For each pulling velocity, five runs were initialized with different starting velocities. The maximum pulling force for each run was extracted from the data. The mean value of that maximum pulling force is used, and the standard deviation of those five runs is used to calculate the error of that data point. The error in E_b was calculated using MATLAB's fit function with weighting factors defined as

$$w_i = \frac{n\left(s_{y_i}\right)^{-2}}{\sum_{i=1}^{n}\left(s_{y_i}\right)^{-2}} \qquad \text{Equation 3}$$

where s_{y_i} is the standard deviation for yi and n is the number of data points. Each data point's contribution to the regression line is inversely proportional to the precision of yi; that is, the more precise the value of y, the greater its contribution to the regression.

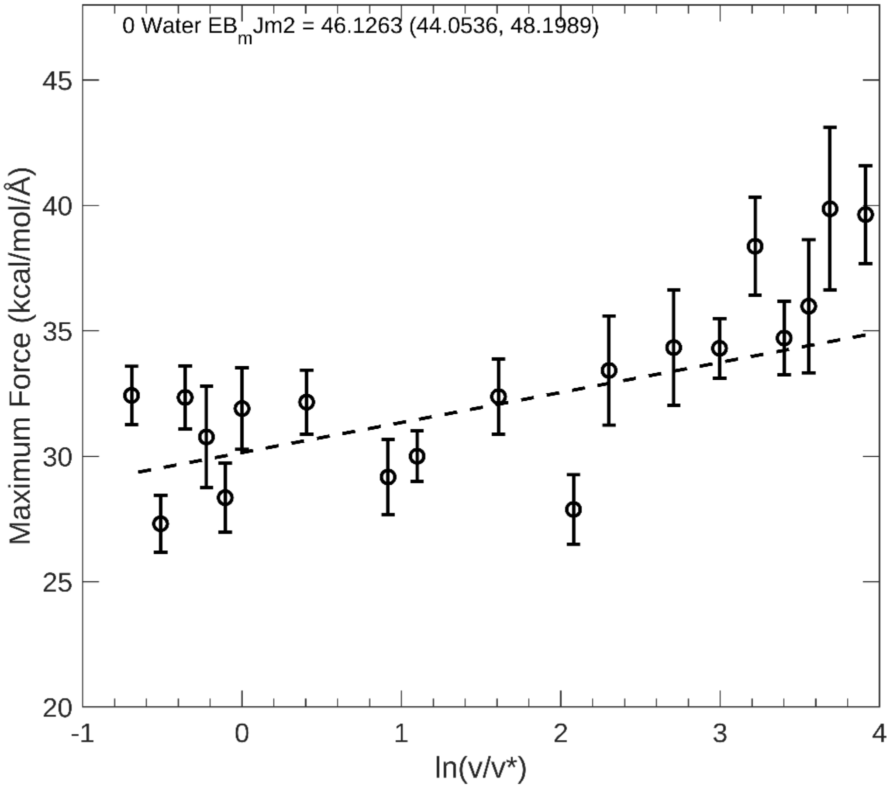

Figure 2. Maximum force vs. ln(v/v*). v* is 1 m/s. Error bars are given as the standard error of 5 runs. Linear fit is used to calculate the bonding energy per area.

Water was incorporated into the simulation using the TIP3P model. Water molecules were placed in an evenly spaced array on the surface of the SiO_2, as shown in Figure 2. The rest of the simulation proceeded in the same manner as the simulations without water. Different amounts of water were added by changing the spacing between water molecules. An example with 100 water molecules added (0.94 water molecules per nm2) is shown in Figure 3. The droplet is above the SiO_2 with water molecules shown in blue. Except for the water molecules, hydrogen atoms are shown in white, carbon atoms in cyan, oxygen in red, sulfur in yellow, nitrogen in blue, and silicon in brown. The simulation is run using periodic boundary conditions so that the SiO_2 surface is pseudofinite.

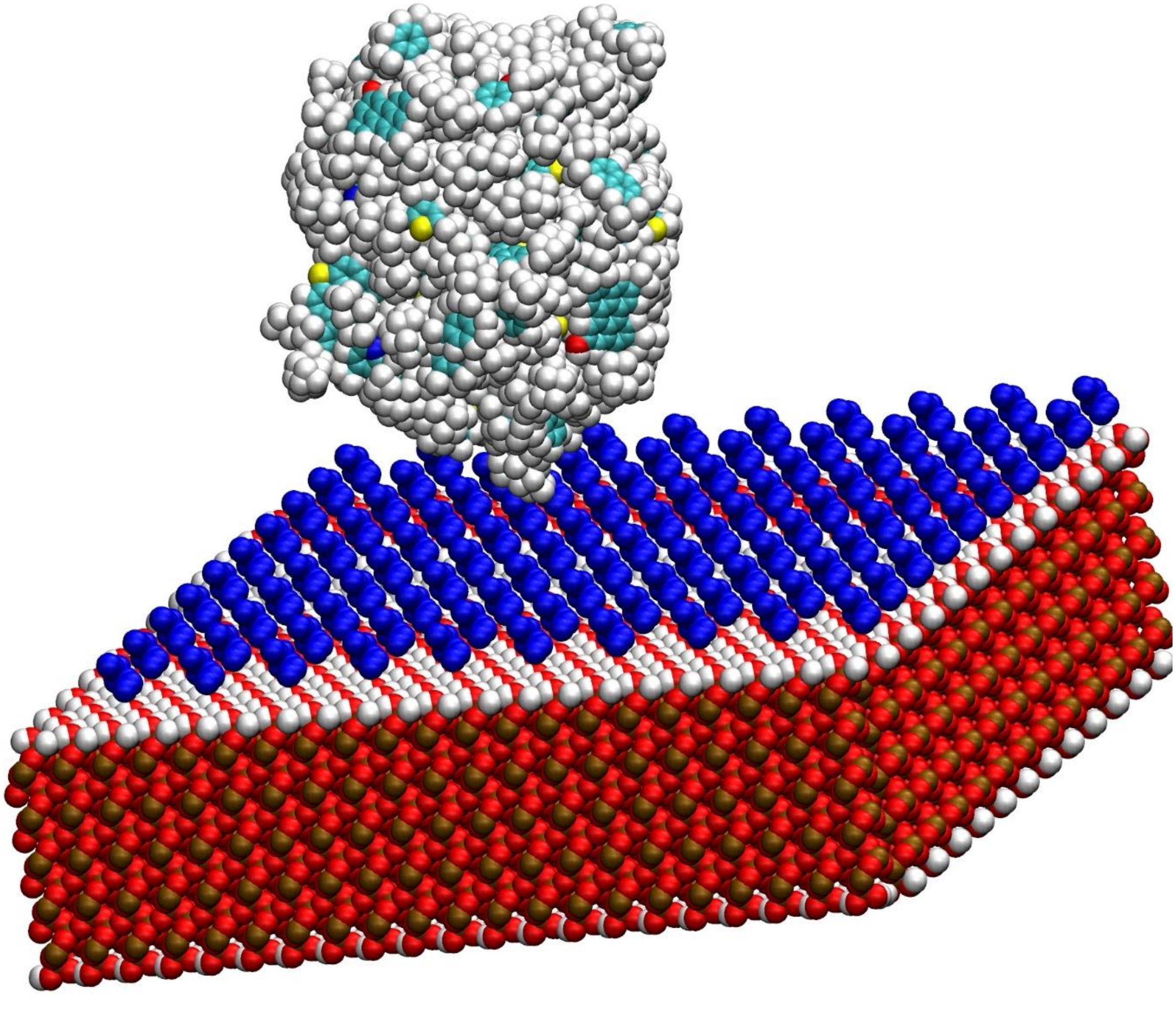

Figure 3. Insertion of water molecules. The asphalt droplet is over the SiO_2 with water molecules (shown in blue) placed above the SiO_2.

Chapter 4. Results and Discussions

In this project, the research team seeks to develop a screening tool for assessment of moisture-induced damage potential of asphalt mixes containing PE. We use Bell's model,[30,33] which relates the pulling velocity and pulling force to the adhesion energy.

To extract the adhesion energy per area, the slope and intercept of the maximum force vs. ln(v/v*) must be extracted (see overview). This is shown for various amounts of added water with the bonding energy shown in text on the plot in Figure 4. Generally, increased water content decreases adhesion energy, though zero water has a lower adhesion energy than ~1 water molecule per nm^2. A few reasons are possible. First, some of the dry tests pulled apart the asphalt droplet rather than simply pulling it off the surface, but this does not happen when water is included. Finally, perhaps a small amount of water promotes hydrogen bonding and increases adhesion, though ultimately, water is detrimental to adhesion, as attested to in the literature.

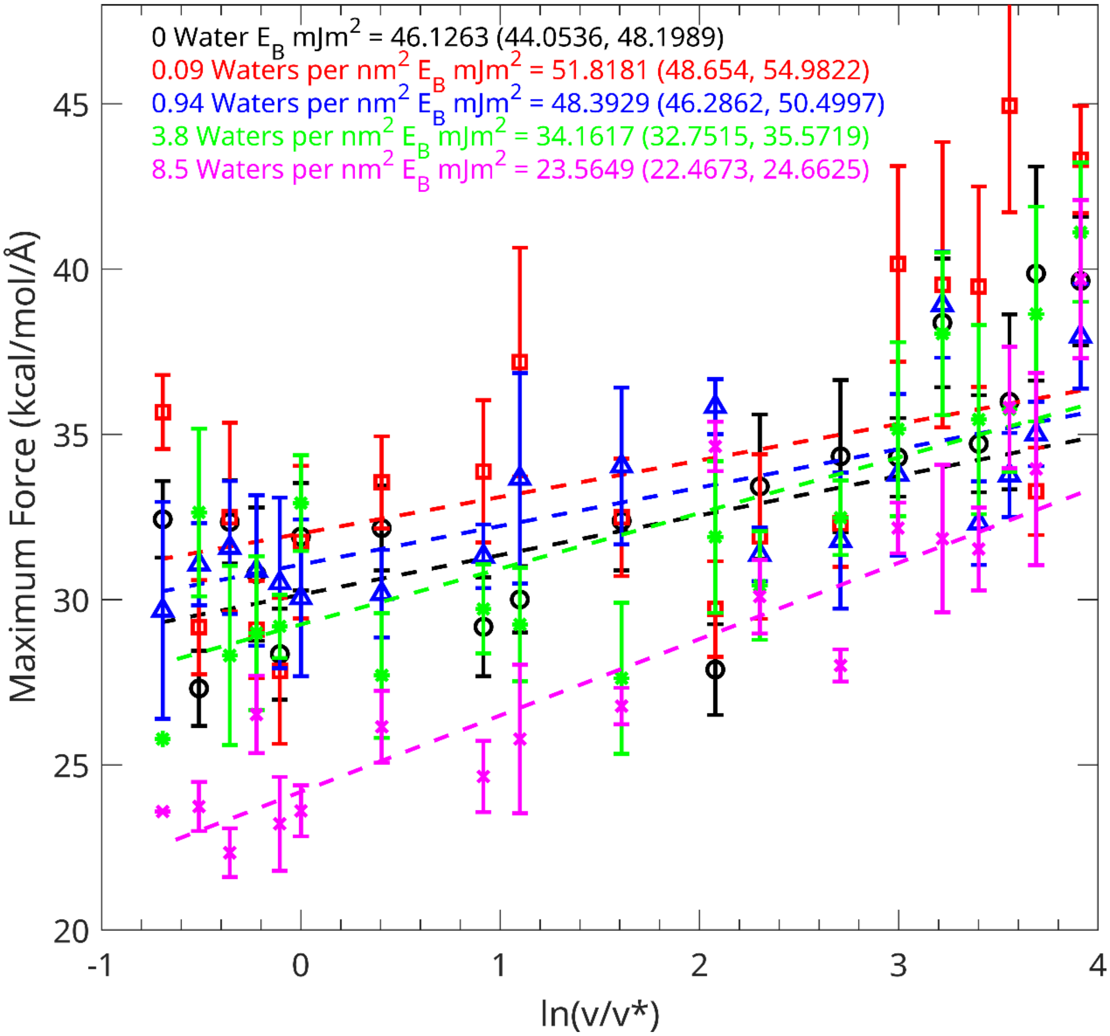

Figure 4. Comparison of adhesion energy vs. water content. 0 water is shown in circles, 0.46 waters per nm^2 is red squares, 0.94 waters per nm^2 in blue triangles, 3.8 waters per nm^2 in green asterisks, and 8.5 waters per nm^2 in magenta xs.

For comparison, experimental measurements give adhesion energy in the range of 30-75 mJ/m^2 under dry conditions depending on the binder, aggregate, and measurement technique. It can be difficult to distinguish between the effect of each between studies. A result of ~46 mJ/m^2 was obtained for dry unmodified asphalt, consistent with experiment. One difficulty in attaining this value is ascertaining the interaction area between the droplet and the aggregate. This was done by taking a snapshot of simulation after good contact was made (that is, just before the droplet was pulled off the surface) and taking the area of the shape containing the droplet atoms in contact with the SiO_2 surface. This gave an area of 282 Å^2 and was fairly consistent between tests (within 12 Å^2 for those sampled). However, the boundary of this shape is not well defined as atoms interact appreciably beyond the hard surface of the LJ (Lennard-Jones) sphere that approximates each atom.

Polymer Addition. Polyethylene was added to the bottom of the asphalt droplet and the calculations were completed, as described previously. A 30-monomer long chain was used. This is shown in Figure 4 and equates to a 2.52 wt% mixture. The droplet has a mass of 32597.393 amu and the polymer has a mass of 843.636 amu.

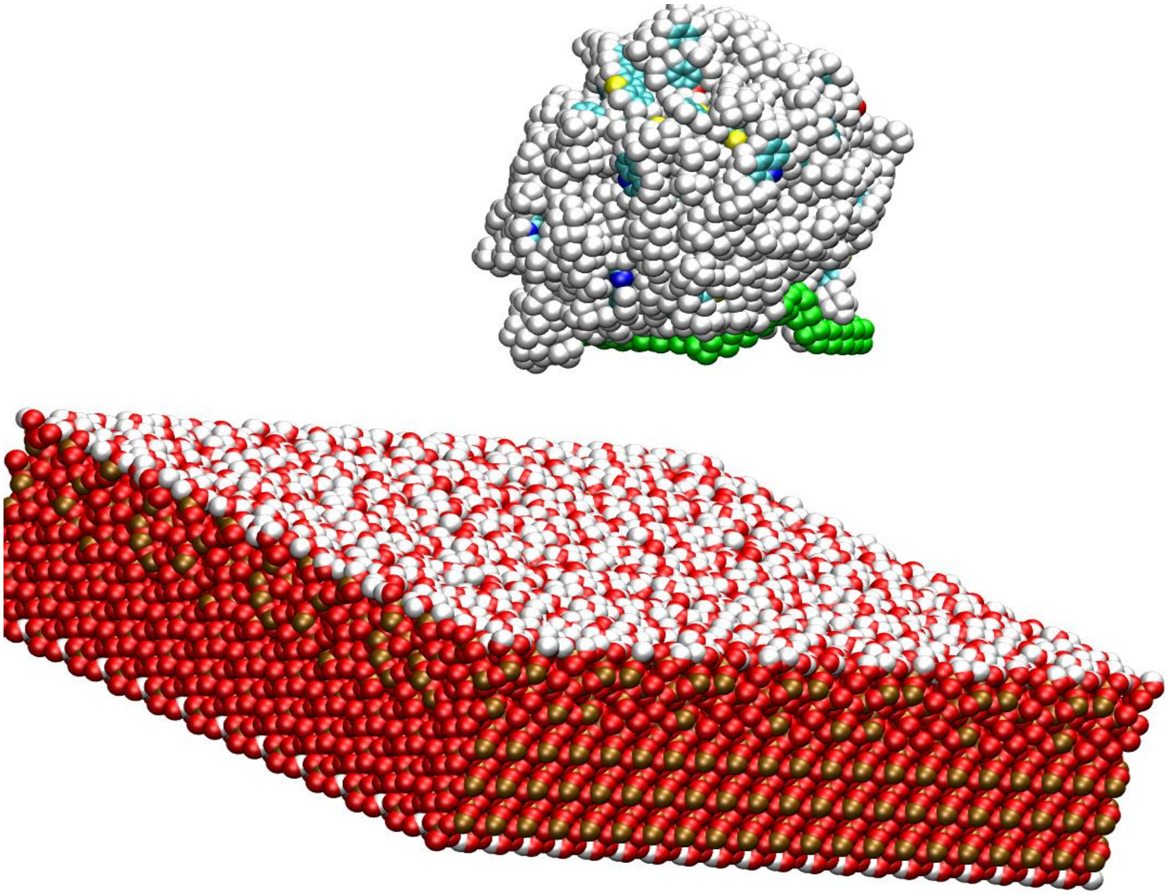

Figure 5. Insertion of PE. Atoms are colored by element: oxygen is red, hydrogen is white, carbon is cyan, sulfur is yellow, nitrogen is blue, and silicon is brown. The polyethylene atoms are colored green to distinguish them from the other asphalt molecules.

Results in the same format as above are shown in Figure 5. The results are qualitatively similar, with a slight increase at low water content, and a decrease at higher water content, but the magnitude and behavior at high water content differ. Comparisons of the binding energy per area are shown in Figure 6.

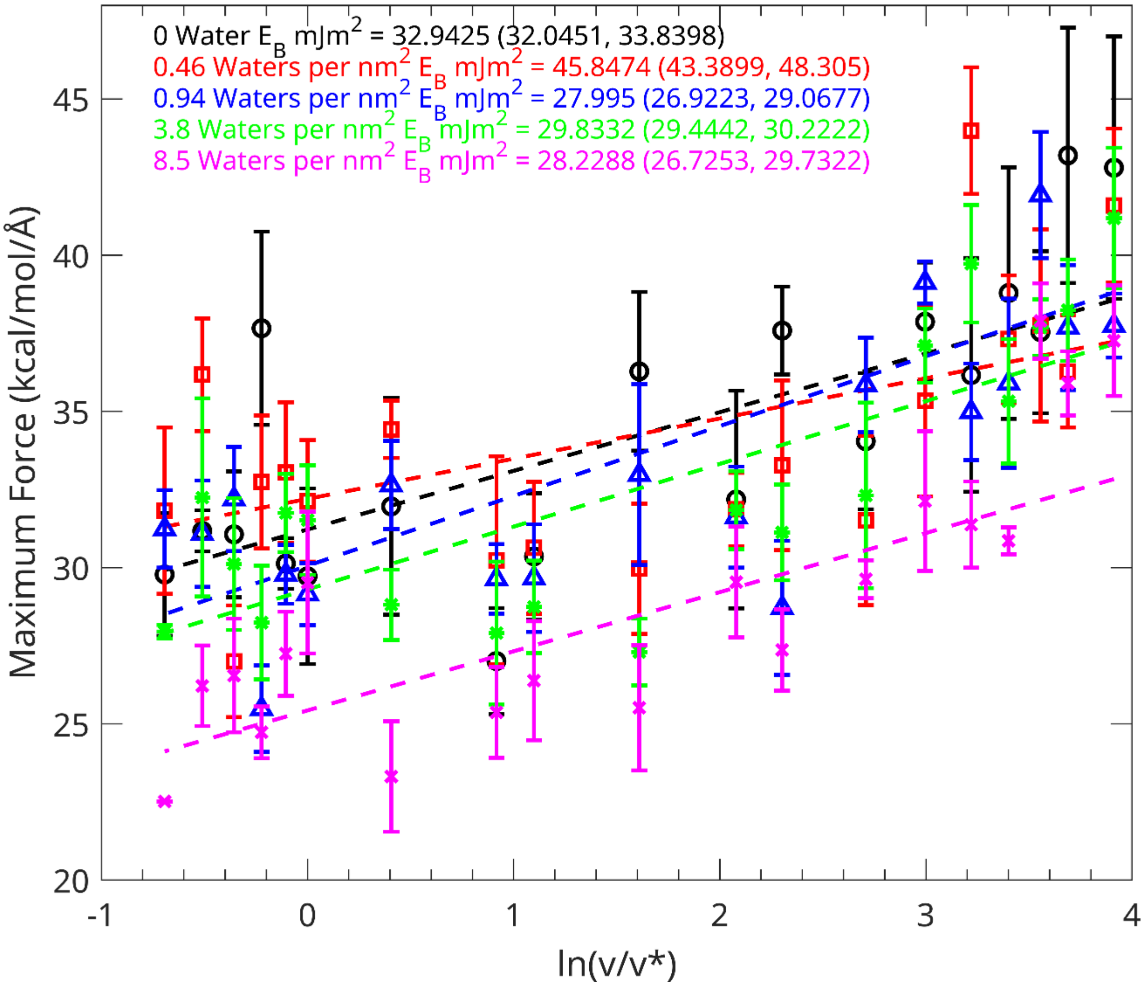

Figure 6. Comparison of adhesion energy vs. water content for 1 PE molecule per droplet (2.52 wt%). 0 water is shown in circles, 0.46 waters per nm^2 is red squares, 0.94 waters per nm^2 in blue triangles, 3.8 waters per nm^2 in green asterisks, and 8.5 waters per nm^2 in magenta xs.

Shown in Figure 6, water significantly impacts the adhesion between binder and silica. Both with and without PE, there is an increase at low water concentrations followed by a decrease in binding energy. This could be caused by increased hydrogen bonding between the asphalt and silica. It could also be caused by an effective increase in the interaction area as the water can act to wet both surfaces. Under dry conditions, the added PE reduces binding energy (46 mJ/m^2 vs. 33 mJ/m^2).

However, at high water content the situation is different. Without PE, the binding energy continues to decrease, potentially leading to premature failure. With PE, the binding energy stabilizes at high water content, indicating that PE could act to induce water damage resistance in the asphalt.

The reduced adhesion under dry conditions when PE is included could be explained by the non-polar nature of PE. It simply has a weaker interaction with SiO_2 than the asphalt which contains some polar components. While not sampled here, it is possible that the PE would spend less time at the surface and mitigate these effects in experimental systems.

The stabilization effect and mitigation of the effect of water could also be explained by the hydrophobic nature of PE. Once in contact with the SiO_2 surface, it may repel water from that surface, thus keeping a dryer overall interaction. This is supported when the trajectories are analyzed. Under dry conditions, the simulations with and without PE look very similar (see Figure 7). However, high water content sometimes results in the PE molecule bridging between the SiO_2 and the asphalt droplet as it moves away. (see Figure 8) Figure 8 presents a visualization of the molecular dynamics simulation immediately following the detachment of the asphalt droplet from the SiO_2 aggregate surface. In this image, water molecules are rendered as a transparent blue surface. The PE allowed the water to be repelled at the interface and a stronger interaction between the droplet (including PE) and the surface was formed. Thus, the relatively weak impact of water on the polymer modifed asphalt. These results suggest that PE could be used to limit the effect of water, though there might be tradeoffs for performance if water is not present. More work is needed.

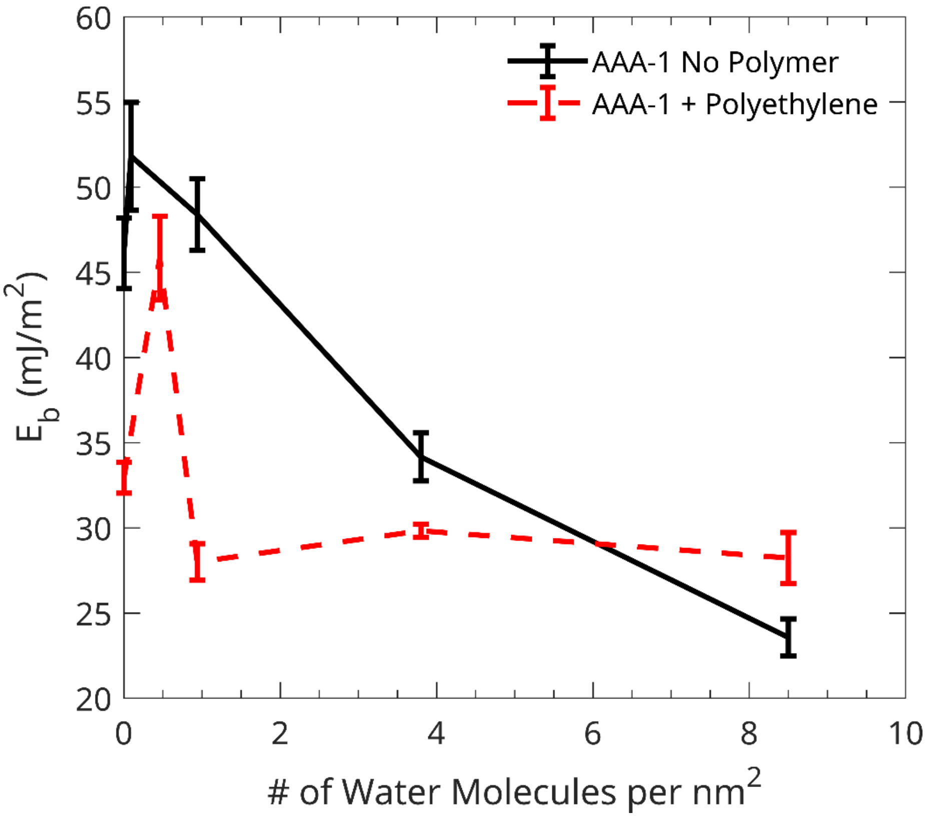

Figure 7. Comparison of adhesion energy vs. water content for no PE vs. PE.

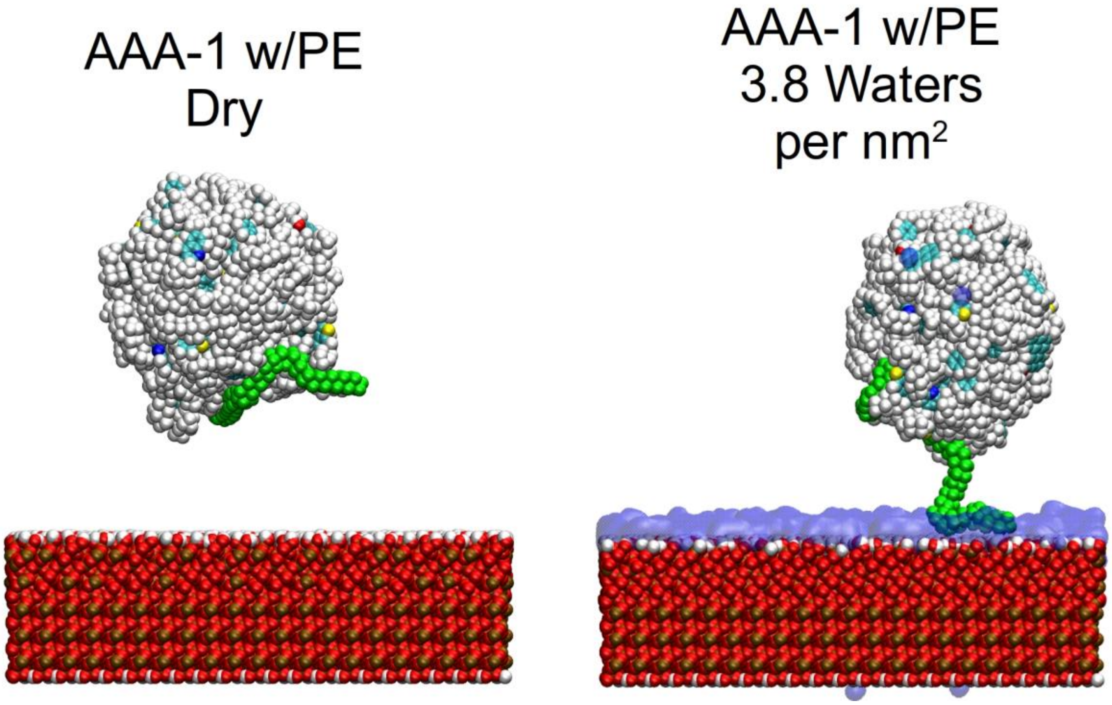

Figure 8. Image of simulation soon after droplet pulloff. Water is shown as a transparent blue surface using the quicksurf method in VMD (Visual Molecular Dynamics).

Chapter 5. Conclusions and Recommendations

This project successfully validated the approach used by achieving dry adhesion energies consistent with experiments (46 mJ/m^2). Interestingly, the study found that at very low water concentrations (<0.5 waters per nm^2), adhesion energy increased. This could be caused by an increase in hydrogen bonding between the binder and aggregate, or potentially by an increased wetting area between binder and aggregate. The first cause would be reflected in experiment, while the second is more of a reflection of the droplet shape on a flat surface.

The addition of polyethylene to the asphalt binder produced two significant effects. First, it reduced the initial dry binding energy from 46 mJ/m^2 to 33 mJ/m^2, likely due to PE's non-polar nature creating weaker interactions with the silica surface compared to the polar components in unmodified asphalt. Second, and perhaps more importantly, PE modification demonstrated a protective effect against water damage at higher water concentrations, with binding energies stabilizing around 28-29 mJ/m^2 rather than continuing to decrease, as observed in unmodified asphalt. This stabilization effect appears to be related to PE's hydrophobic nature, which helps repel water from the asphalt-aggregate interface.

Modification by PE may reduce moisture damage of asphalt in very wet conditions, though the effects it has on dry properties must be studied to ensure those properties are not diminished.

Further work is required in a few areas. First, other modifiers, binders, and aggregate should be tested to see if these effects are universal. Second, the effect of specific placement of the modifier in the droplet, and the typical position of the modifier in the droplet, should be tested. For consistency, the polymer was placed on the bottom of that droplet, but it is unclear exactly where the polymer will partition in general. Coarse-grained simulations could be used to allow sampling of these longer timescale simulations.

Chapter 6. Implementation of Project Outputs

The method has been implemented and validated. Scripts and data files to aid in reproduction and extension of the calculations will be provided on the PI's website (https://www2.latech.edu/~apeters/index.html).

The effect of water at various concentrations on binder to aggregate adhesion was found and reported.

The effect of PE modification to binder and the effects of binder to aggregate adhesion was found and reported. PE reduced the dry adhesion energy but increased wet adhesion energy above the unmodified values. This suggested PE could be used to mitigate water damage, but the effect on dry properties needs to be studied first. The basis for longer studies on the effect of different asphalts or aggregates has been provided.

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Chapter 7. Technology Transfer and Community Engagement and Participation (CEP) Activities

The work of the PI/CoPI was presented at the annual Transportation Research Board meeting in Washington DC in January 2024 and January 2025.

The PI will present the findings in a monthly SPTC webinar.

Chapter 8. Invention Disclosures and Patents, Publications, Presentations, Reports, Project Website, and Social Media Listings

- “Compatibility of Asphalt Binder and Plastic: Simulation and a Thermodynamic Experimental Approach.” Andrew Peters, Nazimuddin Wasiuddin. Invited Talk. Transportation Research Board Annual Meeting, Washington D.C., January 2025.
- “A Thermodynamic Approach to Investigate Compatibility of HDPE, LDPE, and PP Modified Asphalt Binders Using a Novel Differential Scanning Calorimeter (DSC) Method.” Shahjalal Selim, Andrew J. Peters, Nazimuddin Wasiuddin. Transportation Research Board Annual Meeting, Washington D.C., January 2024.
- “A Coarse-Grained Model for Asphalt Binder and Polymer Mixtures Based on the MARTINI Forcefield” Andrew J. Peters. Transportation Research Board Annual Meeting, Washington D.C., January 2024.

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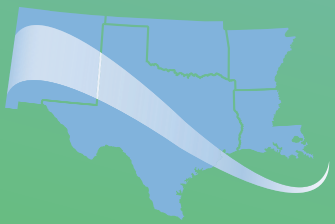

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TRANSPORTATION CENTER

The University of Oklahoma | OU Gallogly College of Engineering
202 W Boyd St, Room 213A, Norman, OK 73019 | (405) 325-4682 | Email: sptc@ou.edu