

# Adsorption Mechanisms of Linear and Branched alkane liquid on solid surfaces that influences Heat Transfer

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## Abstract

The contact interfaces of solid and liquid are common systems in tribology studies where the main parameter looked at are the wear rates and scar. These problems of wear rates and scar are evaluated by adsorption mechanisms. The main contributors of these problems are the character of liquid orientation on solid surfaces that required deep analysis of molecular orientations. Thus, the main purpose of this study is to look at the adsorption mechanisms of liquid on solid surfaces based on the structural quantities of density and orientation order parameters. The simulation system of solid of gold with surfaces of face-centered cubic (FCC) of (100) in contact with three types of alkanes (pentane, heptane and 3-ethyl-pentane) is modeled using molecular dynamics simulations. A uniform temperature is applied throughout the simulation system at 0.7 of the critical temperature of the liquid. It is found that, the adsorption behavior of liquid with linear molecular length is higher as compared to liquid with branches in the molecular, this in away influences the heat transfer near the contact interfaces of solid and liquid. However further investigation is needed to observe the influence of surface structure of the solid surfaces.

*Keywords: solid-liquid interfaces, adsorption mechanisms, liquid alkanes, molecular dynamics simulations.*

## 1. Introduction

Solid-liquid interfaces of solid surfaces in contact with liquid of long polymer have a number of applications in many technological and biological processes such as thermal interface materials [1], energy system [2] tribological system [3], NEMS and MEMS technology [4], and many more. The equilibrium and non-equilibrium properties at the vicinity of solid-liquid interfaces are crucial understanding in nanoscale materials. When the thickness of the polymeric films is in nanometers, macroscopic theory and physics do not work on these films. For these nanoscale systems, the behaviors of the interface are governed by molecular interaction of solid-liquid and surface morphology of the solid [5], [6] which can be summarized as adsorption mechanisms. The knowledge of the adsorption mechanisms denote the understanding of adhesion [7], wetting [8] and lubrication [9]. The adsorption mechanism is closely related with the transport properties of heat and mass transfer.

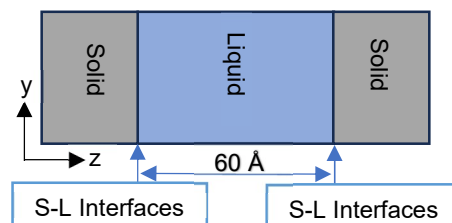
In previous studies, the performance of the adsorption mechanism have been known based on the adsorption of liquid on solid surfaces [10], and the surface morphology of the solid surfaces [8], [11]. However, despite the intense investigation on the adsorption mechanism, the clear insight of the liquid lubricants on the solid surfaces in the molecular level have yet to be explained. Thus, this paper is interested in looking into the adsorption mechanisms in terms of molecular orientation on solid surfaces using non-

equilibrium molecular dynamics simulations. Here three types of alkane liquid (pentane, 3-ethyl-pentane and heptane) in contact with Face-centered Cubic (100) will be evaluated and the adsorption mechanism will be evaluated based on the density, orientation order parameter and radius of gyration.

## 2. Methodology

### 2.1. Layer of solid and liquid and boundary condition

In this simulation the system is arranged in layers of solid, liquid and solid as shown in Fig. 1. The contact interfaces of the solid and liquid is referred to solid-liquid (S-L) interface. Thus, in this simulation there exists two S-L interfaces. The solid is a face-centered cubic (FCC) of (100) surfaces of gold in contact with liquid of pentane, 3-ethyl-pentane and heptane.



**Fig. 1. Layer of solid and liquid of the simulation system**

The overall size of the simulation system is  $40.7 \text{ \AA} \times 40.7 \text{ \AA} \times 114.4 \text{ \AA}$  for the x, y and z-directions. The length of the liquid layer in z-direction is  $60 \text{ \AA}$ . Periodic boundary condition is applied in the x and y-direction of the simulation system. In the z-direction the system is set to be fixed at its position. This setup is due to simulate the conditions of extremely large solid on both sides left and right.

## 2.2. Interaction Forces

In order to replicate the actual solid and liquid, interaction forces are applied to the simulation system. Here there are three interaction forces that needs to be replicated which are the solid-to-solid interaction forces, liquid to liquid interaction forces and solid to liquid interaction forces. The same interaction forces in refs [5], [12] is utilized in this study.

For the liquid-to-liquid interaction forces, there are 2 types of forces utilized to replicate the liquid which are bonded interaction forces and non-bonded interaction forces. The bonded interaction forces consisted of three interaction forces which are stretching interactions, bending interactions, and torsion interactions. As for the non-bonded interaction is the interaction between molecules to molecules or the interaction of atom in the same molecules but are separated by 2 stretching interaction forces also known as the Van Der Waals interaction forces. Here the same interaction forces is applied as in refs [13], [14].

The interaction forces between solid and liquid are replicated by Lorent-Bertholet combining rules. The same interaction forces have been applied in refs [6], [12].

## 2.3. Simulation Details

The reversible reference propagator (r-RESPA) algorithm with multiple times steps is utilized to calculate the position and momenta of the molecules [15]. One femto second and 0.2 femto second respectively for inter and intra molecular interactions were utilized for the time integration time steps.

Initially the simulation was slowly raised to a targeted temperature for 1-to-3-million-time steps. Here the targeted temperature is 0.7 from the critical temperature ( $T_c$ ) of the liquid. Then finally, the temperature of the simulation system was controlled uniformly throughout the simulation system at the  $0.7 T_c$ , for 3-to-5-million-time steps. Throughout this final step, the data acquisition takes place.

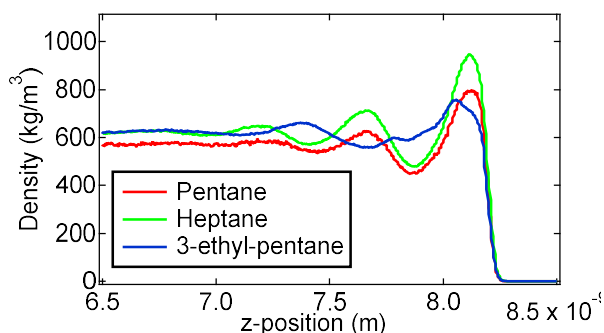
## 3. Result and Discussions

### 3.1. Density

Fig. 1 shows the density distributions of the simulation models. Since the model is symmetric only the left side of the density distributions is shown in the figure. The same density distributions profiles have been observed in previous studies [5], [12], [16], where an oscillation appear near the solid surfaces and a flat line appear at the center of the density distributions. The oscillation nearest to the solid surfaces is referred to as adsorption layer after this.

In this result, it is found that the adsorption layer of heptane and pentane is higher and closer to the solid surface as compared to 3-ethyl-pentane. Based on the

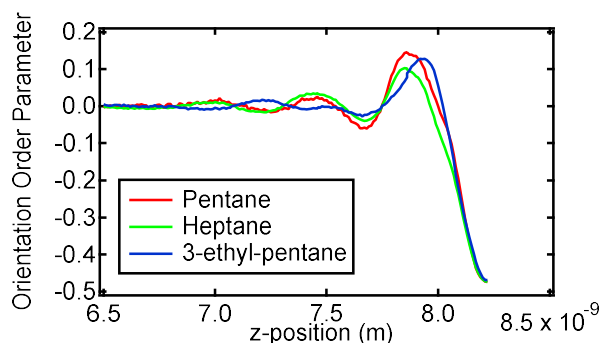
results, peak height of the adsorption layer for heptane is approximately  $945.28 \text{ kg/m}^3$  followed by pentane with the value of  $797.89 \text{ kg/m}^3$  and 3-ethylpentane with the value of  $758.11 \text{ kg/m}^3$ . In addition, the density distribution for 3-ethyl-pentane has differences in the position of the peak and valley. This existence is due to the difference in the molecular structure of the liquid. For pentane and heptane, the molecule structure is a straight line whereas for 3-ethyl-pentane there exist branched exactly at the center of the molecular, thus this branch of molecules in a way influences the behavior of the attraction and repulsion forces. As is well known in past studies [17], [18], the existence of the oscillation near the solid surfaces is due to the attraction and repulsion forces of the liquid and solid molecules. Based on the results it is understood that heptane has the highest adsorption on solid of gold followed by pentane and last, the 3-ethyl-pentane.



**Fig. 2 Density distributions of pentane, 3-ethyl-pentane and heptane.**

### 3.2. Orientation order parameters

Orientation order parameters are used as a references parameter to identify the orientation of liquid on solid surfaces. The value ranges from -0.5 to 1.0 where the -0.5 represents liquid in the perfect parallel to the solid surfaces, 1.0 corresponds to normal to the solid and 0 represents randomly oriented.



**Fig. 3. Orientation order parameter of pentane, 3-ethyl-pentane and heptane.**

Fig. 3 shows the orientation order parameters of pentane, 3-ethyl-pentane, and heptane for the left sides of the simulation model. Based on the results, all of the liquid is in perfect parallel orientation near the solid surfaces and as moves further away from the solid surfaces all the liquid shows a normal orientation to the solid surfaces. The same kind of results have been observed in the past studies [5]. However, there are differences in the position and height of the peaks of the orientation order parameters profiles. Based on the figure it is found that for heptane and

pentane the shape of the profiles is approximately the same however slight differences is observed for 3-ethyl-pentane. Where the peak and valley for the 3-ethyl-pentane is shallow as compared to heptane and pentane. This result shows that although the 3-ethyl-pentane is in parallel to the solid surfaces however it is easily shifted to the random position as it moves further away from the solid surfaces.

#### 4. Conclusion

This study looks into the adsorption behavior of linear and branched liquid. Based on the results, it is understood that liquid with branched liquid is not adsorbed on the solid

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- [10] C. De Recherche, P. Surfaces, and P. Kennedy, "Characterization of Specific Interactions Capacity of Solid Surfaces by Adsorption of Alkanes and Alkenes. surfaces as compared to liquid with linear molecular, thus this factor influenced significantly the character of heat transfer at the interfaces of solid and liquid and hydrodynamics lubrication conditions. Although additional studies needed to look at the contact interfaces of different FCC such as (110) and (111) due to the surface structure effects.

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