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Molecular Modeling and Continuum Analyses of Thin Film Interfaces

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## Abstract

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The combined trends of decreasing application size and increasing requirements for energy efficiency have driven a need for improved understanding and better predictive tools for thin film lubricated systems. Research on such systems is complicated by the involvement of both larger scale phenomena such as fluid flow, material deformation, and material wear, as well as behaviors that are typically only significant on the molecular scale such as solvation pressure, interface slip, and unique thin film fluid properties. Thin film lubricated systems can be investigated by combining traditional lubricated contact models with a molecular scale characterization of thin film behavior. However, this type of integrated research requires a foundation of fundamental understanding of both continuum models for describing a lubricated interface as well as the molecular models that can be used to characterize behaviors of a confined fluid. This dissertation describes the building of that foundation through research performed from the continuum and molecular perspectives individually. Continuum simulation-based studies include formulation of a thermoelastic displacement model with convection, development of a method for rapid prediction of maximum subsurface stress, and evaluation of a mixed elastohydrodynamic lubrication wear model. A molecular simulation that models a lubricated interface was developed and then employed to investigate thin film behaviors and properties including density, solvation pressure, interface slip, and viscosity. Finally, potential areas of overlap between the continuum and molecular models are discussed, and the initial phases of an integration plan for the two models are proposed.

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# Chapter 1 Introduction

## **1.1 Motivation**

In today's society, energy usage is a critical issue to which significant engineering and scientific research is dedicated. One approach to improving energy efficiency is to reduce frictional loses in mechanical systems using lubrication. Frictional losses are minimized in a well designed lubricated system. However, lubricated system design has been complicated in recent years by technological advances that tend towards decreasing size and smaller tolerances, which in turn require thinner lubricating films. The combined trends of decreasing application size and increasing requirements for energy efficiency correspond to a need for better predictive tools in thin film lubricated application design. Thin lubricating films arise in small scale components such as magnetic storage devices or at the interfaces of micro-electro-mechanical systems. In addition, thin film lubrication may also play an important roll in larger-scale applications. For example, there may be local areas of thin film lubrication near regions of surface asperity contact in mixed lubrication. Also, applications lubricated by a thick film during full speed operating are subject to brief periods of thin film lubrication during the critical moments of start up or shut down. The high level goal of this research is to address the need for models that describe thin film lubrication by combining traditional lubricated contact models with molecular simulation-based characterizations of thin film behavior.

Traditional, continuum models used to describe the behavior of tribological systems incorporate contact mechanics, fluid dynamics, and lubricant rheology. Contact mechanics

models the behavior of the contacting solid materials. Fluid dynamics describes flow of the lubricant through the interface. And models that characterize the fluid itself incorporate changes of the lubricant properties as functions of variable contact conditions. However, these models may not be applicable to thin film lubricated systems because molecular scale phenomena may impact the lubricant behavior. A lubricant confined to a thickness comparable to the size of the fluid molecule has been shown to exhibit properties distinct from those of the same fluid in the bulk. Therefore, a simulation of thin film lubrication must incorporate not only traditional lubricated contact models, but also the impact of molecular scale phenomena. As a result, design of applications that operate in the thin film lubrication regime may require predictive tools that integrate both larger-scale effects described using continuum models and molecular-scale effects characterized using atomistic models.

The combination of molecular and traditional contact models requires integration of not only length scales that may differ by several orders of magnitude, but also an interdisciplinary background. Molecular simulation of fluid behavior is predominantly utilized in chemical engineering and related disciplines. However, lubricated contact models are primarily the focus of mechanical engineering research efforts. The thin film lubrication problem requires contribution from both areas. The near term goal of this research is to develop thin film lubrication simulation tools. However, its broader goal is to introduce a multi-scale, interdisciplinary approach to thin film lubrication research.

## 1.2 Approach

The initial phases of this research involve building a foundation for integrated research from the continuum and molecular perspectives individually. This process includes developing familiarity with existing simulation tools as well as modification of some of those tools for application to thin film lubricated systems. Simulation tools utilized in this research include continuum numerical solutions for dry contact, lubricated contact, and material wear, as well as molecular scale Monte Carlo and molecular dynamics simulations. This dissertation primarily describes research done using continuum and molecular models separately. However, in the last chapter, a plan for the initial phases of integration of the two models is introduced.

Chapters 2 through 5 describe contributions to the area of continuum tribological modeling. Although these studies do not directly address the problem of thin film lubrication, they are part of the foundation for integrated research. This includes formulation of a closed form, threedimensional, analytical solution for thermal displacement due frictional heating and convective cooling (Chapter 2); development of a means of rapidly predicting the maximum subsurface stress in rough surface contact using smooth surface approximations of the near surface and global contact stresses (Chapter 3); enhancement of the simplified model developed in Chapter 2 to incorporate the effect of surface roughness using simulation of real rough, sinusoidal, and textured surfaces (Chapter 4); and evaluation of a simulation of material wear in elastohydrodynamic lubrication (EHL) by comparison of simulation predicted trends with experimental observations from the literature (Chapter 5).

Chapters 6 through 10 describe research on thin film behavior performed using molecular simulation tools. First the simulation tool developed for modeling a thin film lubricated interface is described (Chapter 6). Then analyses of individual fluid properties and behaviors are reported. These investigations focus on the behavior thin film density in terms of molecular layering and a decrease of the average density of nano-confined fluids (Chapter 7); analysis of the relationship

between solvation pressure and the distance between a channel wall and the first fluid layer (Chapter 8); investigation of the molecular origins of interface slip from several different perspectives (Chapter 9), and characterization of shear thinning and oscillation of viscosity with film thickness in a thin film under shear (Chapter 10).

Lastly, the initial phases of integration of the continuum and molecular models are introduced. This includes identification of the potential areas where unique thin film behaviors described in Chapters 7 - 10 may have an impact on a lubricated interface modeled using continuum simulation tools such as those presented in Chapters 2 - 5. In addition, as an illustration of the next steps for this research, Chapter 11 presents an analysis of the variation of viscosity due to thin film effects in an EHL interface.

## **Chapter 2**

## A Thermoelastic Displacement Model with Convection

## 2.1 Background

The first continuum model-based investigation will be analysis of the thermoelastic displacement of a surface due to frictional heating and convective cooling. This work is motivated by the significant effect that surface heating has on performance, wear, and failure in many tribological interfaces. Determining the temperature rise of contact interfaces subject to surface heating is essential to predicting thermally induced failures in manufacturing processes and tribology. Frictional heating causes contacting bodies to distort, which in turn affects the contact geometry, pressure distribution, and temperature. The impact on temperature may cause a cycle of frictional heating and temperature rise. Quantification of the effect of frictional heating surfaces (Johnson 1985; Liu and Wang 2001; Liu et al. 2001).

The problem of thermoelastic displacement has been addressed before. Many twodimensional displacement solutions have been developed that do not consider the effect of convective cooling. Solutions of this type were given by (Barber 1971) and (Gladwell and Barber 1983) for an unmoving heat source. Steady state solutions for a moving heat source were given by (Ling and Mow 1965) and (Barber 1972; Barber 1982). Transient solutions for the moving heat source problem were then given by (Barber 1984), (Bryant 1988), (Brock et al. 1997), and (Lee and Ou 2001). Some three-dimensional solutions without the convective effect have also been developed in recent years. Steady state, three-dimensional solutions for a moving heat source were given by (Brock and Rodgers 1997) and by (Lykotrafitis and Georgiadis 2003). Then (Liu et al. 2001) presented a transient solution for this same problem. However, these solutions did not consider the effect of surface cooling due to convection. A solution for thermal displacement with convection was given by (Kulchytsky-Zhyhailo and Yevtushenko 1997). However, this two-dimensional solution was developed for an unmoving heat source only. Solutions for the temperature rise at a surface have progressed more rapidly than the corresponding solutions for thermal displacement. For example, (DesRuisseaux and Zerkle 1970), (Fischer et al. 2001), and (Liu et al. 2004) calculated evaluated temperature rise due to a moving heat source and convection. In particular, the DesRuisseau and Zerkle result was analytical, three-dimensional, and allowed for an unsteady heat source. However, none of these solutions were applied to thermal displacement.

This chapter presents the development of a closed form, three-dimensional, analytical solution for thermal displacement due frictional heating and convective cooling based on the expression for temperature rise given by (DesRuisseaux and Zerkle 1970) and the thermoelastic displacement analysis of (Liu et al. 2001). Some of the content of this chapter is also available in (Martini et al. 2005).

### 2.2 Problem Description

The normal thermal displacement that occurs at the interface of two contacting surfaces may be modeled as a semi-infinite body subject to transient frictional heating and convective cooling. This model is schematically illustrated in Figure 2-1.



Figure 2-1: Description of the physical domain and coordinates and variables; spatial coordinates  $(x_1, x_2, x_3)$ , heat flux (q), and time (t).

The frictional heating at the contact area is represented by a local heat source. The heat flux is determined from a heat partition analysis by which the amount of heat flowing into each contacting surface is calculated (Liu et al. 2001). The convective term is assumed to act everywhere on the surface of the half-space. The convection rate is assumed to be constant and have a uniform heat transfer coefficient.

#### 2.3 Formulation

The uncoupled governing partial differential equations for transient heat conduction and quasi-static thermoelastic deformation ( $u_i$  = displacement in the *j* direction) are (Liu et al. 2001):

$$k\Delta T_{,ii} = \frac{\partial}{\partial t} (\Delta T); \quad C_{ijkl} u_{k,lj} = (3\lambda + 2\mu)\alpha \Delta T_{,i}$$
(2.1)

The material properties utilized in the above expression are defined in Table 2-1. The temperature and thermoelastic boundary conditions for the surface are (Liu et al. 2001; Liu et al. 2004):

$$-k\rho c\Delta T_{,3} = q$$
, within surface heating area  
 $k\rho c\Delta T_{,3} = hT$ , outside surface heating area  
 $C_{ijkl}u_{k,l}n_j = (3\lambda + 2\mu)\alpha\Delta Tn$ , everywhere  
(2.2)

An expression for normal displacement due to a temperature change was given as Equation 5 in (Liu et al. 2001). This result was formulated using the equations for elasticity, thermal displacement, and Green's functions presented by (Mura 1998).

$$u_{3}(x_{1}, x_{2}, x_{3} = 0, t) = \frac{\alpha(1+\nu)}{\pi} \int_{\xi_{3}=0}^{\infty} \int_{\xi_{2}=-\infty}^{\infty} \int_{\xi_{1}=-\infty}^{\infty} \frac{-\xi_{3}\Delta T}{\left[(x_{1}-\xi_{1})^{2}+(x_{2}-\xi_{2})^{2}+\xi_{3}^{2}\right]^{3/2}} d\xi_{1} d\xi_{2} d\xi_{3}$$
(2.3)

An analytical expression for the temperature distribution due to a point source that incorporates the effect of surface convection was given as Equation 4 in (DesRuisseaux and Zerkle 1970). This expression is indeed the Green's function. When a distributed heat source is at the surface of the half-space, i.e.  $at(x'_1, x'_2, x'_3 = 0)$ , the corresponding expression for temperature at a location of  $(\xi_1, \xi_2, \xi_3)$ , and time *t*, becomes the following:

$$\Delta T = \int_{t'=0}^{t} \int_{x_{2}^{'}=-\infty}^{\infty} \int_{x_{1}^{'}=-\infty}^{\infty} \frac{q(x_{1}^{'}, x_{2}^{'})}{\rho c} e^{-\left[\frac{\left[(\xi_{1}-x_{1}^{'})-V(t-t')\right]^{2}+(\xi_{2}-x_{2}^{'})^{2}}{4k(t-t')}\right]} \left\{\frac{1}{4[\pi k(t-t')]^{3/2}} \left[e^{\frac{-\xi_{3}^{2}}{4k(t-t')}}\right] - \frac{h}{k^{2}\rho c 4\pi(t-t')} erfc\left[\frac{\xi_{3}}{2\sqrt{k(t-t')}} + \frac{h\sqrt{t-t'}}{\sqrt{k}\rho c}\right] e^{\frac{\xi_{3}h}{k\rho c} + \frac{h^{2}(t-t')}{k(\rho c)^{2}}} dx_{1}^{'} dx_{2}^{'} dt'$$
(2.4)

Here, erfc() is the complementary error function. The second term in the brackets in the above equation is due to surface convection. Equations 2.3 and 2.4 can be combined to yield an expression for normal displacement due to frictional heating and convective cooling. The following change of variables should be made,

$$\gamma_{1} = x_{1}^{'} - \xi_{1}$$

$$\gamma_{2} = x_{2}^{'} - \xi_{2}$$

$$\Delta t = t - t^{'}$$
(2.5)

Then define the following as the main part of the integral kernel,

$$A = \int_{\xi_{3}=0}^{\infty} \left\{ \left[ \frac{1}{4\rho c (\pi k \Delta t)^{\frac{3}{2}}} \right] e^{\left[ \frac{-\xi_{3}^{2}}{4k\Delta t} \right]} - \frac{h}{4(\rho c)^{2} \pi k^{2} \Delta t} e^{\left[ \frac{\xi_{3}h}{k\rho c} + \frac{h^{2} \Delta t}{k(\rho c)^{2}} \right]} erfc \left[ \frac{\xi_{3}}{2\sqrt{k\Delta t}} + \frac{h\sqrt{\Delta t}}{\rho c\sqrt{k}} \right] \right\}$$

$$\int_{\xi_{2}=-\infty}^{\infty} \int_{\xi_{1}=-\infty}^{\infty} \frac{-\xi_{3}}{(\gamma_{1}^{2} + \gamma_{2}^{2} + \xi_{3}^{2})^{\frac{3}{2}}} e^{\left[ \frac{\left[ (\xi_{1}-x_{1}^{'})-V\Delta t-\gamma_{1} \right]^{2} + (\xi_{2}-x_{2}^{'}-\gamma_{2})^{2}}{4k\Delta t} \right]} d\xi_{1} d\xi_{2} d\xi_{3}$$
(2.6)

Using this expression and substituting Equation 2.3 for temperature distribution into Equation 2.4 for displacement yields the following,

$$u_{3}(\mathbf{x}_{1}, \mathbf{x}_{2}, \mathbf{x}_{3} = 0, t) = \frac{\alpha(1+\nu)}{\pi} \int_{t'=0}^{t} \int_{x'_{2}=-\infty}^{\infty} \int_{x'_{1}=-\infty}^{\infty} (qA) dx_{1}' dx_{2}' dt'$$
(2.7)

The integrals with respect to  $\xi_1$  and  $\xi_2$  in A can be evaluated by performing a double Fourier transform in two dimensions. This is possible by observing that the double integral is a 2D convolution with the substitution of  $\tau_1 = x_1 - V\Delta t - x_1'$  and  $\tau_2 = x_2 - x_2'$ . The transform is performed using the convolution theorem and the following expressions (Campbell and Foster 1931; Morrison 1994). Note that  $\tilde{f}^{j}$  indicates a Fourier transform of the function f in the j direction,  $\int_{-\infty}^{\infty} f(x_j) e^{-iw_j \cdot x_j} dx_j$  and  $w_j$  is the frequency coordinate in the j direction

$$f(x, y, z) = \frac{1}{2\pi} \frac{z}{(x^2 + y^2 + z^2)^{3/2}} \Leftrightarrow \widetilde{f}^{x, y} = e^{-z\sqrt{w_1^2 + w_2^2}}$$
(2.8)  
$$f(x) = e^{-ax^2} \Leftrightarrow \widetilde{f}^x = \sqrt{\frac{\pi}{a}} e^{-\frac{w^2}{4a}}$$
$$f(x - x_0) \Leftrightarrow e^{-iwx_0} \widetilde{f}^x \qquad \text{with } x_0 = V\Delta t$$

The two-dimensional Fourier transform of *A* can be separated into two parts – one due to the heat source,  $\widetilde{A}_{heatsource}^{x,y}$ , and the other due to the surface convection,  $\widetilde{A}_{convection}^{x,y}$ . That is,

$$\widetilde{A}^{x,y} = \widetilde{A}^{x,y}_{heatsource} + \widetilde{A}^{x,y}_{convection}$$
(2.9)

where

$$\widetilde{A}_{heatsource}^{x,y} = \frac{-2\sqrt{\pi}}{\rho c \sqrt{k\Delta t}} e^{-k\Delta t w'^2} \int_{\xi_3=0}^{\infty} e^{\left[\frac{-\xi_3}{4k\Delta t}\right]} e^{-\xi_3 \sqrt{w_1^2 + w_2^2}} d\xi_3,$$
  

$$\widetilde{A}_{convection}^{x,y} = \frac{2\pi h}{(\rho c)^2 k} e^{-k\Delta t w'^2} \int_{\xi_3=0}^{\infty} e^{\left[\frac{\xi_3 h}{k\rho c} + \frac{h^2 \Delta t}{k(\rho c)^2}\right]} e^{-\xi_3 \sqrt{w_1^2 + w_2^2}} erfc \left[\frac{\xi_3}{2\sqrt{k\Delta t}} + \frac{h\sqrt{\Delta t}}{\rho c\sqrt{k}}\right] d\xi_3,$$
  
and  $w' = \sqrt{w_1^2 + w_2^2 + iw_1 V/k}$ .

The integrals over  $\xi_3$  in the above expressions can be evaluated analytically using the following relationships:

$$\frac{2}{\sqrt{\pi}} \int_{z}^{\infty} e^{-y^{2}} dy = \operatorname{erfc}(z)$$

$$\int e^{bz} \operatorname{erfc}(az) = \frac{1}{b} \left[ e^{bz} \operatorname{erfc}(az) - e^{\frac{b^{2}}{4a^{2}}} \operatorname{erfc}\left(\frac{b}{2a} - az\right) \right]$$
(2.10)

After performing the integration, the normal displacement becomes the following.

$$u_{3}(\mathbf{x}_{1}, \mathbf{x}_{2}, \mathbf{x}_{3} = 0, t) = \frac{(1+\nu)\alpha}{\pi} IFT^{x, y} \left( \int_{t'=0}^{t} \widetilde{q}^{x, y} (\widetilde{A}_{heatsource}^{x, y} + \widetilde{A}_{surface}^{x, y}) dt' \right)$$
(2.11)

where

$$\widetilde{A}_{heatsource}^{x,y} = \frac{-2\pi}{\rho c} e^{-iw_1 V \Delta t} erfc \left[ \sqrt{k \Delta t (w_1^2 + w_2^2)} \right]$$

and

$$\widetilde{A}_{convection}^{x,y} = \frac{2\pi h}{k(\rho c)^2 \left(\frac{h}{\rho c} - \sqrt{w_1^2 + w_2^2}\right)} e^{\left[-k\Delta tw^{\prime 2} + \frac{2h\Delta t}{\rho c}\sqrt{w_1^2 + w_2^2} - \frac{h^2\Delta t}{k(\rho c)^2}\right]} \begin{cases} e^{k\Delta t \left(\frac{h}{\rho c} - \sqrt{w_1^2 + w_2^2}\right)^2} \\ e^{k\Delta t} \left(\frac{h}{\rho c} - \sqrt{w_1^2 + w_2^2}\right) \end{cases} e^{\frac{2h\Delta t}{\rho c} \left(\frac{h}{\rho c} - \sqrt{w_1^2 + w_2^2}\right)} e^{rfc} \left[\frac{h\sqrt{\Delta t}}{\rho c\sqrt{k}}\right] \end{cases}$$

Here,  $IFT^{x,y}$  is the inverse Fourier transform in two dimensions. The result is a general, analytical expression for normal surface displacement due to a heat source and convective cooling.

## 2.4 Sample Application

To illustrate the possible applications of this result, a specific case will be examined in detail. The case analyzed will be that of a non-moving, constant (over time) heat source. Using the notation presented in this paper, this case is defined as:

$$V = 0; \quad q \neq q(t) \tag{2.12}$$

The general solution for displacement, Equation 2.11, can be applied to this case by moving the heat flux outside the time integral. Then, the normal surface displacement for this specific case becomes

$$u_{3}(x_{1}, x_{2}, x_{3} = 0, t) = \frac{(1+\nu)\alpha}{\pi} IFT^{x,y} \left( \widetilde{q}^{x,y} \int_{t'=0}^{t} (\widetilde{A}^{x,y}_{heatsource} + \widetilde{A}^{x,y}_{convection}) dt' \right).$$
(2.13)

At this point, several new variables will be introduced to simplify the expression resulting from integration over time. First, the time integrated expressions for  $\widetilde{A}_{heatsource}^{x,y}$  and  $\widetilde{A}_{convection}^{x,y}$  will be denoted by  $\widetilde{B}_{heatsource}^{x,y}$  and  $\widetilde{B}_{convection}^{x,y}$ , respectively. Then, *a*, will be used to replace the frequently occurring function of transformed variables,  $\sqrt{w_1^2 + w_2^2}$ . Note that  $w' = \sqrt{w_1^2 + w_2^2 + iw_1V/k}$  is equal to *a* in this case. And finally, the following substitutions will be made for products of the material constants:

$$b_{1} = \frac{2ah}{\rho c} (1-k) + \frac{h^{2}}{(\rho c)^{2}} \left(k - \frac{1}{k}\right)$$

$$b_{2} = \frac{h}{\rho c \sqrt{k}} - \frac{h\sqrt{k}}{\rho c} + a\sqrt{k}$$

$$b_{3} = -ka^{2} + \frac{h^{2}}{(\rho c)^{2}} \left(2 - \frac{1}{k}\right)$$

$$b_{4} = \frac{h}{\rho c \sqrt{k}}$$

$$(2.14)$$

The time integral can be analytically evaluated using the following relationships:

$$\int_{0}^{t} erfc(a\sqrt{t'})dt' = (t)erfc(a\sqrt{t}) - \frac{\sqrt{t}}{a\sqrt{\pi}}e^{-a^{2}t} + \frac{1}{2a^{2}}erf(a\sqrt{t})$$

$$\int_{0}^{t} erfc(b_{2}\sqrt{t'})e^{b_{1}t'}dt' = \frac{1}{b_{1}} \left[ erfc(b_{2}\sqrt{t})e^{b_{1}t} + \frac{b_{2}}{b_{1}\sqrt{b_{2}^{2} - b_{1}}}erf\left(\sqrt{b_{2}^{2} - b_{1}}\sqrt{t}\right) - 1 \right]$$
(2.15)

The resulting solution for normal displacement in the case of a non-moving, constant heat source is the following:

$$u_{3}(x_{1}, x_{2}, x_{3} = 0, t) = \frac{2(1+\nu)\alpha}{\rho c} IFT^{x, y} \left\{ \widetilde{q}^{x, y} \left( \widetilde{B}^{x, y}_{heatsource} + \widetilde{B}^{x, y}_{convection} \right) \right\}$$
(2.16)

where

$$\widetilde{B}_{heatsource}^{x,y} = (-t) \operatorname{erfc}(a\sqrt{kt}) + \frac{\sqrt{t}}{a\sqrt{\pi k}} e^{-ka^2t} - \frac{\operatorname{erf}(a\sqrt{kt})}{2ka^2}$$

and

$$\widetilde{B}_{convection}^{x,y} = \frac{h}{k(h-\rho ca)} \left\{ \frac{1}{b_1} \left( e^{b_1 t} \operatorname{erfc} \left[ b_2 \sqrt{t} \right] + \frac{b_2}{\sqrt{b_2^2 - b_1}} \operatorname{erf} \left[ \sqrt{b_2^2 - b_1} \sqrt{t} \right] - 1 \right) - \frac{1}{b_3} \left( e^{b_3 t} \operatorname{erfc} \left[ b_4 \sqrt{t} \right] + \frac{b_4}{\sqrt{b_4^2 - b_3}} \operatorname{erf} \left[ \sqrt{b_4^2 - b_3} \sqrt{t} \right] - 1 \right) \right\}$$

This expression can be used to directly solve for the transient surface displacement with no numerical integration required. The solution is elegant, simple and easy to apply. It should be noted that the square root term may become negative. In this case, the error function is replaced by the complex scaled complementary error function (cerfe) in FORTRAN 90 library IMSL®.

For example, if 
$$b_2^2 - b_1 < 0$$
, then  $\frac{b_2}{\sqrt{b_2^2 - b_1}} erf\left[\sqrt{b_2^2 - b_1}\sqrt{t}\right]$  becomes  
 $\frac{b_2 i}{\sqrt{b_1 - b_2^2}} \left(1 - e^{-t(b_1 - b_2^2)} cerfe\left[\sqrt{b_1 - b_2^2}\sqrt{t}\right]\right).$ 

The steady state solution for this case can be obtained by taking the limit of Equation 2.16 as time goes to infinity. This is calculated using the infinity limit of the error function of one, and the infinity limit of the complementary error function of zero. The simplified steady state solution is then the following:

$$u_{3}(x_{1}, x_{2}, x_{3} = 0, t \to \infty) = \frac{2(1+\nu)\alpha}{\rho c k} IFT^{x, y} \left\{ \tilde{q}^{x, y} \left[ \frac{-1}{2a^{2}} + \frac{h}{(h-\rho ca)} \left( \frac{b_{2}}{b_{1}\sqrt{b_{2}^{2}-b_{1}}} - \frac{1}{b_{1}} - \frac{b_{4}}{b_{3}\sqrt{b_{4}^{2}-b_{3}}} + \frac{1}{b_{3}} \right) \right] \right\}$$

$$(2.17)$$

Using this result, the steady state solution for the non-moving, constant heat source case can be easily and accurately calculated.

Integration over time was performed analytically for the specific case described in this section. However, the general solution given in Equation 2.11 can be applied to many other situations. Specifically, the authors believe that a solution for a moving, constant heat source could be obtained analytically using an approach similar to that given in this section. However, the analysis of this case was not completed for this work. In addition, it is anticipated that the time integration could be performed for a general heat source either by numerical integration or possibly with an additional Fourier transform in time. Using a convolution with respect to time, the general solution given in Equation 2.11 would become:

$$u_{3}(x_{1}, x_{2}, x_{3} = 0, t) = \frac{(1+\nu)\alpha}{\pi} IFT^{x, y} \left\{ IFT^{t} \left\{ q^{x, y, t} \left( \widetilde{A}_{heatsource}^{x, y, t} + \widetilde{A}_{convection}^{x, y, t} \right) \right\} \right\}$$
(2.18)

As will be discussed in the next section, the transforms and inverse transforms can be performed using highly efficient and accurate numerical methods.

#### 2.5 Numerical Results and Discussion

The solution for the special case of the non-moving, constant heat source was implemented as a computer simulation. Numerical results can be used to graphically illustrate the surface displacement due to a heat source and convective cooling. This requires performing an inverse Fourier transform in two dimensions. The inverse transform was done numerically using the discrete convolution and fast Fourier transform method (DC-FFT) presented in (Liu et al. 2000). The DC-FFT method is accepted as being both efficient and accurate.

In this example, the solution will be used to simulate thermal displacement at the interface of point contact between a ball and an equivalent half-space. The material parameters are similar to those used in (Liu and Wang 2001). The material properties of both the ball and the flat are assumed to be those of typical carbon steels. These properties are summarized in Table 2-1.

Property	Value	Units
heat capacity, <i>c</i>	4.6x10 <sup>8</sup>	mm²/s²/ºC
thermal diffusivity, <i>k</i>	3.45	mm²/s
thermal expansion coefficient, $\alpha$	1.55x10⁻⁵	/°C
Poisson's ratio	0.3	-
density, <i>p</i>	7.85x10 <sup>-6</sup>	kg/mm³
Surface heat conduction coefficient, h	0 to 1000	W/m²/ºC

Table 2-1: Material parameters used in the numerical simulation.

The surface heat transfer coefficient, h, is a function of the material properties of the solids, the properties of the surrounding fluid, and the operating conditions. For the examples given in this paper, the surface heat transfer coefficient is varied from 1 to 1000 W/m<sup>2</sup>/°C. This range of values includes most experimentally measured heat transfer coefficients for an unmoving heat

source. Surface heat transfer coefficients measured for convection in ambient air have been found to be on the order of 10  $W/m^2/^{\circ}C$  (Jayamaha et al. 1996). However, for convection in a water mist, the heat transfer coefficient has been found to be significantly higher on the order to 1000  $W/m^2/^{\circ}C$  (Sozbir et al. 2003).

The calculation domain is 1mm by 1mm in size and discretized into  $64\times64$  elements. However, the Fourier domain used in the simulation is eight times larger than the actual contact domain in order to minimize error introduced at the boundaries. The center of the ball corresponds to the center of the discretized contact domain. Contact is then simulated by calculating the Hertzian contact pressure distribution and applying a heat source with the same distribution. The heat source distribution used in this example was  $10^9 \sqrt{1-4r^2}$  W/m<sup>2</sup>, where r is the radial distance from the center of contact.

Due to that axi-symmetric nature of this problem, the three-dimensional solution in  $x_1$ ,  $x_2$ ,  $x_3$  space that was obtained from the simulation can be represented in two dimensions. Figure 2-2 illustrates this by presenting the same solution in two dimensions and three dimensions.



Figure 2-2: The normal displacement  $(-u_3)$  at 0.5 seconds shown equivalently in two and three dimensions: (a) three-dimensional, (b) two-dimensional.

To facilitate analysis and comparison, most simulation results will be presented twodimensionally on half of the  $x_1, x_3$  plane.

When the surface heat transfer coefficient, h, is zero, the displacement solution given in Equation 2.16 reduces to a solution for thermal displacement due to frictional heating only (i.e. no convection). Figure 2-3 illustrates the solution for normal surface displacement due to frictional heating only at times increasing from 0.05 to 5 seconds.



Figure 2-3: The normal surface displacement (- $u_3$ ) due to frictional heating only (i.e. no convection) shown at t = 0.05, t = 0.1, t = 0.5, t = 1 and t = 5 seconds.

This solution for h = 0 was compared to that obtained by Liu et. al. for displacement due to frictional heating only (Liu et al. 2001). The solutions were found to be the same, therefore partially validating the simulation results presented in this paper.

The convective effect is incorporated into the solution by choosing a non-zero value for the surface heat transfer coefficient. The normal displacement due to both frictional heating and convective cooling at increasing time for a surface heat transfer coefficient of 1000  $W/m^2/^{\circ}C$  is presented in Figure 2-4.



Figure 2-4: The normal surface displacement (- $u_3$ ) due to frictional heating and convection ( $h = 1000 \text{ W/m}^{2/\circ}\text{C}$ ) shown at t = 0.05, t = 0.1, t = 0.5, t = 1 and t = 5 seconds.

It can be observed that the normal displacement increases with time. However, once time has continued long enough, the shape of the displacement result changes only minimally while the magnitude increases monotonically. This behavior indicates an approach to steady state and has been observed in previous studies of the steady state thermal displacement due to an axi-symmetric, unmoving heat source (Barber 1971; Gladwell and Barber 1983). The steady state shape of the displacement in this research can be evaluated by adjusting the long time results to a reference point. This is illustrated in Figure 2-5 for a reference point at the outside edge of the displacement.



Figure 2-5: The normal thermal displacements (- $u_3$ ) with convection ( $h = 1000 \text{ W/m}^2/^{\circ}\text{C}$ ) at 5 and 10 seconds adjusted to a reference point at the edge of the displacement.

It can be observed from Figure 2-5 that the normalized solutions at 5 and 10 seconds are nearly equal. The average percent difference between the adjusted solutions at these two times is less than 1%. Therefore, it can be interpreted that the solution has reached nearly steady state at 5 seconds.

Next, the effect of convection will be demonstrated by evaluating solutions with and without convection, and the effect of the surface heat transfer coefficient. Figure 2-6 shows displacement solutions at 5 seconds for surface heat transfer coefficients of  $h = 0, 1, 10, 100, 500, \text{ and } 1000 \text{ W/m}^{2/\text{o}}\text{C}.$ 



Figure 2-6: Comparison of the normal surface displacement  $(-u_3)$  after 5 seconds with no convection and convection where  $h = 1, 10, 100, 500, \text{ and } 1000 \text{ W/m}^{2/\circ}\text{C}$ .

These results indicate that a larger heat transfer coefficient corresponds to less normal displacement. However, it appears that the effect is not significant for smaller values of h. This is illustrated more clearly in Figure 2-7 which contains a plot of the percent that the displacement at the center of contact is reduced due to convective cooling for various heat transfer coefficients.



Figure 2-7: Percent that normal displacement at the center of contact is reduced due to convective cooling,  $\% = (|u_{3,heatsource}| - |u_{3,convection}|)/(|u_{3,heatsource}|) \times 100$ , after 5 seconds as a function of the surface heat transfer coefficient.

It can be seen from this plot that convection decreases the thermal displacement by less than 2% unless the heat transfer coefficient is greater than approximately  $100 \text{ W/m}^{2/\circ}\text{C}$ . As was noted previous, large heat transfer coefficients are not typical for convection in ambient, unmoving air (Jayamaha et al. 1996). Therefore, the effect of convection may not be a significant factor in solutions to problems under these conditions. However, for fast moving air, or for a water mist, the heat transfer coefficient may be much larger and the effect of convection on thermal displacement solutions may become important (Sozbir et al. 2003).
The effect of time is also considered. It was observed that the effect of surface cooling for large heat transfer coefficients was to reduce the normal surface displacement. As illustrated in Figure 2-8, this effect increases with time. Figure 2-8 shows the percent of contact center displacement reduction due to convection for h = 10, 100, and 1000 W/m<sup>2</sup>/°C as a function of time.



Figure 2-8: Percent that normal displacement at the center of contact is reduced due to convective cooling,  $\% = (|u_{3,heatsource}| - |u_{3,convection}|)/(|u_{3,heatsource}|) \times 100$ , for h=10, 100 and 1000 W/m<sup>2</sup>/°C as time increases from 0.05 to 5 seconds.

It can be seen that the effect of surface cooling is more significant at longer times. To summarize, the results of this example case for a constant, unmoving heat source indicate that the effect of convection on normal surface displacement is more significant for larger heat transfer coefficients and at longer times. This is expected since convective cooling affects the rate of temperature rise, and therefore the displacement.

## 2.6 Conclusions

A three-dimensional, transient solution for normal surface displacement due to a heat source and convective cooling has been developed. A closed form, analytical solution is formulated for the general case. Then the general solution is applied to a specific case to illustrate how the result might be used. This specific case is implemented as a computer simulation of the normal, surface displacement due to a constant, non-moving, Hertzian distributed heat source and convective cooling. Results of the simulation indicate that convective cooling decreases thermal displacement and that this effect is strongly dependant on the surface heat transfer coefficient.

# Chapter 3 Rapid Prediction of Maximum Stress, Part I

## 3.1 Background

In this chapter, the scope of dry surface contact investigations is expanded to the critical area of subsurface stress prediction. Understanding and anticipating the effects of surface roughness on subsurface stress in the design phase can help ensure that performance and life requirements are satisfied. One approach used to address this problem is to simulate contact between digitized real surfaces. Although many statistical models for surface generation have been developed and used for contact simulation, direct digitization of real surfaces may yield the most realistic description of surface characteristics (Liu et al. 1999). For the contact simulation, elastic-perfectly plastic models are often employed. These models have been shown to result in an overestimate of asperity stiffness. However, they are still frequently used because of the relative simplicity of the numerical formulation and their computational efficiency (Mihailidis et al. 2001).

Many research efforts have investigated the effect of surface roughness on subsurface stress using numerical simulation (Bailey and Sayles 1991; Lubrecht and Ioannide 1991; Yu and Bhushan 1996; Palasantzas and De Hosson 2000; Mihailidis et al. 2001; Tao et al. 2001; Gong and Komvopoulos 2003; Kadiric et al. 2003). Understanding this effect is particularly important for prediction of such near-surface failure mechanisms as spalling, pitting, or micro-pitting (Bailey and Sayles 1991; Mihailidis et al. 2001; Kadiric et al. 2003) This research continues the investigation of surface roughness and stress via simulation of contact between real, digitized

surfaces using an elastic-perfectly plastic model. The results of the simulations are evaluated in order to predict the magnitude and location of maximum stress. Trends are identified which enable quick estimation of the simulation results based on surface discretization, operating conditions, and material properties. The numerical source of these trends is evaluated in order to develop a standard method for predicting the results of an elastic-perfectly plastic contact simulation. These estimations can be used as an effective and efficient tool for rapid prediction of maximum subsurface stress for real surface contact. Some of the content of this chapter is also available in (Martini et al. 2006).

### **3.2 Contact Simulation Details**

A set of fifty nine real machined surfaces were digitized using a white light interferometer. A summary of the surface types and the range of root-mean-square  $(R_q)$  values measured for each type is given in Table 3-1.

 Table 3-1:
 Summary of real machined surfaces digitized and then used for contact simulation

Description	Surfaces	Minimum <i>Rq</i> (µm)	Maximum <i>Rq</i> (µm)
Ground	29	0.265	1.213
Honed	8	0.383	0.716
Polished	2	0.151	0.156
Shaved	14	0.175	0.948
Turned	6	0.317	0.763

These surfaces differ not only by roughness height but also by texturing. To illustrate the differences the various surfaces evaluated, contour plots of selected ground, honed, and polished surfaces are shown in Figure 3-1.



Figure 3-1: Digitizations of selected ground (Rq=1.14  $\mu$ m), honed (Rq=0.70  $\mu$ m), and polished (Rq=0.15  $\mu$ m) surfaces (from top to bottom) illustrating differences in surfaces texturing.

Surface texturing or patterning has been shown to significantly impact contact pressure and subsurface stress distributions (Bailey and Sayles 1991; Yu and Bhushan 1996; Tao et al. 2001; Gong and Komvopoulos 2003; Kadiric et al. 2003).

Each of the fifty nine surfaces was used in a contact simulation of dry, frictionless point contact. The simulation model is illustrated in Figure 3-2.



Figure 3-2: Model of dry, frictionless point contact used in the simulations.

The material properties, operating conditions, and numerical parameters for the simulation are summarized in Table 3-2.

Parameter			Value	Units
Reduced Radius, R			0.01	m
Equivalent $1/E' = (1 - v^2)/E = (1$	Young's $v^2 \rangle / E$	Modulus,	109.89x10 <sup>9</sup>	Ра
Pressure Limit, $P_{lim}$			2033x10 <sup>6</sup>	Ра
Load, W			1 to 900	Ν
Discrete unit size in the plane of contact, $dx = dy$			7.08x10 <sup>-6</sup>	m
Discrete unit size in the direction of the load, dz			5.00x10 <sup>-7</sup>	m

**Table 3-2: Summary of the simulation parameters** 

The elastic-perfectly plastic contact model used here is the same as that described by the authors in a previous publication (Liu and Wang 2001). However, in this case the simulations are of isothermal contact and therefore do not incorporate the thermal displacement effect. Basically, the logic performed by the simulation code is to satisfy the constraints of zero pressure where there is no contact, pressure between zero and a pressure limit at contact points, and load balance. Plasticity is simulated by not allowing the pressure to exceed a pressure limit. The pressure limit,  $P_{lim}$ , is chosen to be three times the yield strength of steel, above which it is expected that the material will plastically deform (Lee and Ren 1996; Mihailidis et al. 2001).

The simulation utilized the discrete convolution-fast Fourier transform algorithm (Liu et al. 2000) and the single-loop conjugate gradient method (Polonsky and Keer 1999) for accurate and efficient numerical calculation. The discretization scheme and corresponding notation are shown in Figure 3-3.



Figure 3-3: Discretization used in the simulation in the direction of the applied load (left) and the plane of contact at  $z=z_l$  (right).

The subsurface stress distribution corresponding to the surface pressure is computed using a Green's function approach (Johnson 1985; Liu and Wang 2002). The continuous form of the relationship between stress and normal pressure is given as

$$\sigma_{qr}(x,y,z) = \iint p(\xi,\eta) g_{N,qr}(x-\xi,y-\eta,z) d\xi d\eta$$
(3.1)

The discrete form of this equation, that defines the stress in terms of the pressure and a set of influence coefficients,  $D_{N,qr}^{i-\xi,j-\eta,l}$  is given as

$$\sigma_{qr}(x_i, y_j, z_l) = \sum_{\xi} \sum_{\eta} P(x_{\xi}, y_{\eta}) D_{N,qr}^{i-\xi, j-\eta, l}$$
(3.2)

If a new function is introduced,  $T_{N,qr}(x,y,z) = 2\pi \int_{\xi=0}^{x} \int_{\eta=0}^{y} g_{N,qr}(\xi,\eta,z) d\xi d\eta$ , the following

expression for the influence coefficients is obtained

$$D_{N,qr}^{i-\xi,j-\eta,l} = \frac{1}{2\pi} \begin{bmatrix} T_{N,qr}(x_i - x_{\xi} + \frac{dx}{2}, y_j - y_{\eta} + \frac{dy}{2}, z_l) \\ + T_{N,qr}(x_i - x_{\xi} - \frac{dx}{2}, y_j - y_{\eta} - \frac{dy}{2}, z_l) \\ - T_{N,qr}(x_i - x_{\xi} + \frac{dx}{2}, y_j - y_{\eta} - \frac{dy}{2}, z_l) \\ - T_{N,qr}(x_i - x_{\xi} - \frac{dx}{2}, y_j - y_{\eta} + \frac{dy}{2}, z_l) \end{bmatrix}$$
(3.3)

These functions can be evaluated for an uncoated elastic half-space using the Boussinesq solutions.

$$\begin{cases} T_{N,xx}(x,y,z) = -2\nu \arctan\left(\frac{xy}{R_s z}\right) + 2(1-2\nu) \arctan\left(\frac{x}{R_s + y + z}\right) - \frac{xz}{R_s(R_s + y)} \\ T_{N,yy}(x,y,z) = T_{N,xx}(y,x,z) \\ T_{N,xz}(x,y,z) = \frac{-z^2}{R_s(R_s + y)} \\ T_{N,zz}(x,y,z) = -\arctan\left(\frac{xy}{R_s z}\right) + \frac{xz}{R_s(R_s + y)} + \frac{yz}{R_s(R_s + x)} \\ T_{N,xy}(x,y,z) = (2\nu - 1) \ln(R_s + z) - \frac{z}{R_s} \\ T_{N,yz}(x,y,z) = \frac{-z^2}{R_s(R_s + x)} \\ R_s = \sqrt{x^2 + y^2 + z^2} \end{cases}$$
(3.4)

When z is zero,  $\arctan\left(\frac{xy}{R_s z}\right) = \frac{\pi}{2} sign(xy)$ . Here, the von Mises stress will be used for analysis.

The von Mises stress is calculated from the principal stresses  $\sigma_1, \sigma_2$  and  $\sigma_3$  using the following expression

$$\sigma_{VM} = \sqrt{\frac{1}{6} \left[ (\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2 \right]}$$
(3.5)

The von Mises stress is often calculated in contact analyses because it can be used to predict yield according to the von Mises yield criterion, which has been found to match experimental results for metallic contact better than other yield theories (Bhushan 1999).

#### 3.3 Results and Analysis

### 3.3.1 Stress as a Function of Depth

Often the focus of a stress field analysis is on the magnitude and location of the maximum stress because failure has been found to be initiated at stress concentrations (Kadiric et al. 2003). The analyses presented here are based on the maximum von Mises stress in each plane below the surface as a function of the plane depth. Figure 4 illustrates the relationship between the commonly reported centerline stress distribution and an analysis of the location and magnitude of the maximum von Mises stress.



Figure 3-4: Relationship between a typical real rough surface centerline stress distribution and the corresponding analysis of maximum stress as a function of depth.

This example is for the case of a honed surface subject to a 300 N load. For clarity the axes of the plot will be rotated such that the maximum stress is given on the vertical axis and the depth on the horizontal axis. This representation of the subsurface stress will be used for most of the analyses presented.

The subsurface stress distribution was analyzed at loads ranging from 1 to 900 N for each of the real, rough surfaces. The maximum value of the von Mises stress in each plane parallel to the surface as a function of plane depth is illustrated in Figure 3-5 for applied loads of 100, 300, and 900 N.



Figure 3-5: Range of the maximum subsurface stress as a function of depth below the surface for all surfaces evaluated at applied loads of 100, 300, and 900 N.

The shaded region indicates the range of results obtained for all of the real surfaces evaluated. It was found that the shape of the stress distribution range changed as the load increased. However, the maximum value was always at a depth of 3  $\mu$ m below the surface and had a magnitude of around 780 MPa which is 115% of the material yield strength. As has been observed before by other researchers, the depth and magnitude of maximum stress were found to be independent of applied load (Mihailidis et al. 2001).

The choice of discretization in the direction of loading, dz, is important when evaluating the location of maximum stress. If the discretization is too large, the stress peak just below the surface will not be discernable. For example, if dz is chosen to be 6 µm, a maximum stress at 3 µm will not be found. Therefore, to obtain an accurate representation of the location of the maximum stress, it is necessary to use a discretization small enough to identify the near surface stresses.

#### 3.3.2 Near Surface Stress

It is well known that stress peaks occur near the surface due to asperity contact (Bailey and Sayles 1991; Lubrecht and Ioannide 1991; Yu and Bhushan 1996; Mihailidis et al. 2001; Kadiric et al. 2003). In addition, the results obtained in this research indicate that the maximum stress is always at the same depth and has about the same magnitude. In order to explain this consistency, the relationship between the pressure distribution and the maximum stress is evaluated. For the three example ground, honed, and polished surfaces (texturing illustrated in Figure 3-1), the pressure distributions corresponding to an applied load of 300 N are shown in Figure 3-6.



Figure 3-6: Pressure distributions for selected ground, honed, and polished surfaces (from top to bottom) with location of maximum stress indicated by a circle.

The location of the maximum von Mises stress in the x-y plane is indicated by a circle. In these three cases, and for all other surfaces and applied loads evaluated in this research, the maximum

stress was found to correspond to a location near the edge of the contact at the pressure limit. This can be explained by an analysis of the stress calculation and the effect of using a pressure limit.

A closer look at the local pressure distribution around the point of maximum stress reveals that the maximum stress corresponds to a small area (usually only one discrete square) at the pressure limit surrounded by a zero pressure zone, as illustrated in Figure 3-7.



Figure 3-7: Local pressure distribution around the location of the maximum stress (center square). This illustrates the trend of observing the maximum stress at a small area at the pressure limit surrounded by a zero pressure zone.

A local pressure distribution at the pressure limit can be approximated by a disk of constant pressure,  $P_{lim}$ , with radius *a*. The corresponding stress field can then be calculated from Equations 3.2, 3.3, and 3.4. In cylindrical coordinates,  $\sigma_{xx}$ ,  $\sigma_{yy}$  and  $\sigma_{zz}$ , this is

$$\begin{pmatrix} \sigma_{rr} & 0 & 0\\ 0 & \sigma_{\theta\theta} & 0\\ 0 & 0 & \sigma_{zz} \end{pmatrix}$$
 where 
$$\begin{cases} \sigma_{rr} = \sigma_{\theta\theta} = -p_0 \left[ \frac{1+2\nu}{2} - \frac{(1+\nu)}{\left(1+\frac{a^2}{z^2}\right)^{\frac{1}{2}}} + \frac{1}{2\left(1+\frac{a^2}{z^2}\right)^{\frac{3}{2}}} \right]$$
(3.6) 
$$\sigma_{zz} = -p_0 \frac{1}{\left(1+\left(\frac{z}{a}\right)^2\right)^{\frac{3}{2}}}$$

The von Mises stress is then calculated from the components of this stress tensor as  $\sigma_{VM} = \sqrt{\frac{1}{3} ((\sigma_{rr} - \sigma_{zz})^2)}$ .

A single discrete unit square  $(dx^*dx)$  can be approximated by a disc of radius  $a_s = (dx/2)\sqrt{2}$ . This radius also corresponds to the size of the minimum significant asperity. The stress distribution for this disc at constant pressure  $P_{lim}$  calculated using Equation 3.6 is illustrated in Figure 3-8.



Figure 3-8: Stress distribution corresponding to a disc approximating a single discrete unit square of constant pressure at the pressure limit.

For the surface discretization used in this research, the maximum stress occurs at a depth of 3  $\mu$ m, which is the same depth as was observed for the rough surface simulations. Since the rough surface maximum stress was found at a small area at the pressure limit surrounded by a zero pressure zone in all cases, this analysis explains its occurrence at the same depth of 3  $\mu$ m.

The next consideration is why the maximum stress is found at these small, isolated areas at the pressure limit. Consider the continuous form of the influence coefficients for a surface *S*.

$$\sum_{(i,j)\in S} D_{N,qr}^{i,j,l} \approx \iint_{S} g_{N,qr}(\xi,\eta,z) d\xi d\eta$$
(3.7)

For the case of unidirectional loading considered here, the shear components of the stress (offdiagonal components of the tensor) are much less than the normal components.

$$\forall (i, j, k) \in [1, 3]^3, i \neq j \Rightarrow \left| \iint_{S} g_{N, ij}(\xi, \eta, z) d\xi d\eta \right| << \left| \iint_{S} g_{N, kk}(\xi, \eta, z) d\xi d\eta \right|$$
(3.8)

Using this relationship, an approximation can be made that the stress corresponding to the pressure limit is

$$\underline{\underline{\sigma}} = \iint_{S} P_{\lim} \underline{\underline{T}_{N}(\xi, \eta, z)} d\xi d\eta \approx P_{\lim} \iint_{S} \begin{pmatrix} g_{N,xx} & 0 & 0 \\ 0 & g_{N,yy} & 0 \\ 0 & 0 & g_{N,xx} \end{pmatrix} d\xi d\eta$$
(3.9)

Assuming  $\sigma_{xx} = \sigma_{yy}$  due to the absence of friction, the von Mises stress is calculated as

$$\sigma_{VM}(0,0,z) = \sqrt{\frac{1}{6} \left( \left( \sigma_{xx} - \sigma_{yy} \right)^2 + \left( \sigma_{yy} - \sigma_{zz} \right)^2 + \left( \sigma_{zz} - \sigma_{xx} \right)^2 \right)} = \frac{1}{\sqrt{3}} \left| \sigma_{xx} - \sigma_{zz} \right| (3.10)$$

Using the x-y symmetry of S and the fact that the direction of the loading is always down

$$\sigma_{VM}(0,0,z) \approx \frac{P_{\text{lim}}}{\sqrt{3}} \left( \iint_{S} g_{N,xx}(\xi,\eta,z) d\xi d\eta - \iint_{S} g_{N,zz}(\xi,\eta,z) d\xi d\eta \right)$$
(3.11)

This expression indicates that the stress in any layer below the surface can be approximated as the sum of the local stress contributions.

Assume that surface *S* consists of three components,  $S_1$ ,  $S_2$ , and  $S_3$  such that  $i \neq j \Rightarrow S_i \cap S_j = \emptyset$  and  $S = S_1 \cap S_2 \cap S_3$ . The outer diameter of  $S_1$ ,  $S_2$ , and  $S_3$  are one discrete unit, three discrete units, and five discrete units respectively. This theoretical surface is illustrated in Figure 3-9.



Figure 3-9: Illustration of theoretical surface S consisting of three rings of different radii.

The expression for the influence coefficients for the stress at the center of S is

$$\int_{S} g_{N}(\xi,\eta,z) d\xi d\eta = \int_{S_{1}} g_{N}(\xi,\eta,z) d\xi d\eta + \int_{S_{2}} g_{N}(\xi,\eta,z) d\xi d\eta + \int_{S_{3}} g_{N}(\xi,\eta,z) d\xi d\eta$$
(3.12)

Using this relationship, the stress field for the operating conditions and material properties listed in Table 2 can be calculated. If the three discs comprising *S* were separate (*S*<sub>1</sub>, *S*<sub>1</sub>+*S*<sub>2</sub>, *S*<sub>1</sub>+*S*<sub>2</sub>+*S*<sub>3</sub>) and at the pressure limit, the individual stress contributions at the center of *S* and at a depth of 3  $\mu m$  can be calculated using Equation 3.6. The results of this calculation are  $\sigma_{VM}^{dx/2} = 777MPa$ ,  $\sigma_{VM}^{3dx/2} = 563MPa$ , and  $\sigma_{VM}^{5dx/2} = 443MPa$ . Therefore, when *S*<sub>1</sub>, *S*<sub>2</sub>, and *S*<sub>3</sub> are all at the pressure limit, the total stress is  $\sigma_{VM}^{S} = \sigma_{VM}^{dx/2} + (\sigma_{VM}^{3dx/2} - \sigma_{VM}^{dx/2}) + (\sigma_{VM}^{5dx/2} - \sigma_{VM}^{3dx/2}) = \sigma_{VM}^{5dx/2} = 443 MPa$ . However, if *S*<sub>2</sub> has zero pressure, the stress is  $\sigma_{VM}^{S} = \sigma_{VM}^{dx/2} + (\sigma_{VM}^{5dx/2} - \sigma_{VM}^{3dx/2}) = 563 MPa$ . Two observations things can be made from this example. First, the smaller the size of a region at the pressure limit, the larger the individual stress contribution. And second, a zero pressure zone surrounding an area at the pressure limit has the effect of increasing the overall von Mises stress. This gives us an explanation of the location in the x-y plane of the maximum von Mises stress observed in the simulated contact of real surfaces. It can be concluded that the maximum stress will always be found at a small, isolated contact at the pressure limit.

Analysis of the correlation between maximum stress and the pressure limit leads to consideration of the likelihood that some part of the pressure distribution will be at the pressure limit. A single asperity contact that is at the minimum discernable size of one discrete unit can be approximated by a Hertz contact between a ball of radius  $R_s = (dx/2)\sqrt{2}$  and a half-space. The Hertz relationship between pressure and load (Bhushan 1999) can be used to predict the load at which the contact will reach the pressure limit.

$$P_0 = \left(\frac{6WE'^2}{\pi^3 R^2}\right)^{\frac{1}{3}} \Longrightarrow W_{\text{lim}} = \frac{\pi^3 R^2 P_{\text{lim}}^3}{6E'^2}$$
(3.13)

For the material properties used in this analysis and  $R = R_s = (dx/2)\sqrt{2}$ , the limiting load is  $9.01 \times 10^{-5}$  N. Based on this value, it is expected that the pressure limit will be reached at a single asperity even for small load cases. It has been demonstrated using plasticity index critierion and results from purely elastic simulations that the asperities on most engineering surfaces can plastically deform even under very light loads (Sayles 1996). This was verified in the present work for loads as small as 1 N using the full elastic-perfectly plastic contact simulation. For all surfaces and loads considered, some part of the contact area was at the pressure limit.

In the previous sections, the depth and magnitude of the near surface maximum stress were shown to be functions of the size of the corresponding isolated asperity. In this case, asperity size was limited by the spatial resolution of the surface digitization instrument. However, if the asperity size is changed, so too will be the maximum von Mises stress. This was illustrated in simulations of 2D elastic contact between surfaces with controlled micro-roughness wavelength (Bucher 2006). In real surface contact, however, there is a lower limit to the size of asperities that significantly affect the subsurface stress distribution. This is because very small surface features are subject to extremely high stresses and therefore plastic deformation. Criteria for identifying minimum significant roughness size have been developed (Bucher 2006). But frequently, in simulations run during the design of engineering applications, the surface discretization is taken to be the same as the profile sampling interval (Sayles 1996).

## 3.3.3 Global Contact Stress

Using the analysis in the previous section, the location and approximate magnitude of the maximum stress distribution near the surface can be predicted from the results of a constant pressure disc analyses. However, the maximum stress distribution far below the surface must also be considered. It is expected that the stress due to the global shape (as opposed to local asperity contacts) of a rough surface contact will be similar to that of smooth surface contact (Bailey and Sayles 1991; Lubrecht and Ioannide 1991). The stress distribution for smooth surface contact can be predicted using Hertz theory (Johnson 1985). The stress tensor corresponding to the Hertz pressure distribution is given in Equation 3.14.

$$\begin{pmatrix} \sigma_{rr} & 0 & 0\\ 0 & \sigma_{\theta\theta} & 0\\ 0 & 0 & \sigma_{zz} \end{pmatrix}$$
 where 
$$\begin{cases} \sigma_{rr} = \sigma_{\theta\theta} = -p_0 \left[ \left[ 1 - \frac{z}{a} \tan\left(\frac{a}{z}\right) \right] + \frac{1}{2 \times \left(1 + \left(\frac{z}{a}\right)^2\right)} \right] \\ \sigma_{zz} = -p_0 \frac{1}{1 + \left(\frac{z}{a}\right)^2} \end{cases}$$
(3.14)

This Hertz stress distribution can be compared to the rough surface stress distribution below the location of the Hertz maximum at 0.48*a*.

Figure 3-10 shows a comparison between the maximum stress distribution simulated for the real rough surfaces and the Hertz predicted distribution (Equation 3.14).



Figure 3-10: Maximum stress distributions at 100, 300, and 900 N loads for the real, rough surfaces (range shown in grey) and the Hertz predicted distribution (black line). Diagonal patterned region indicates depths below the Hertz maximum.

The diagonal patterning identifies depth below the Hertz predicted maximum where the results are expected to be comparable. From these plots it can be observed that the Hertz predicted stress distribution at depths below the location of the maximum correlates well with the upper bound of the real surface stress range for 100 and 300 N cases. However, the Hertz stress is significantly higher for the 900 N load case. These results indicate that the Hertz stress is a good approximation for the upper bound of real surface stress at smaller loads, but the solutions diverge at larger loads. This divergence is due to the material yield and the applied pressure limit. If elastic behavior is assumed, the maximum Hertz pressure with a 900 N load is 2761 *MPa*. That is nearly one and a half times greater than pressure limit used in the elastic-perfectly-plastic model.

For larger loads, a better approximation to the stress distribution far below the surface can be obtained from a model in which the entire contact area is at the pressure limit. The formulation is similar to that detailed previously for the case of a single discrete square. However, in this case, the radius of contact is  $a_G = (3WR/4E')^{\frac{1}{3}}$  instead of  $a_S = (dx/2)\sqrt{2}$ . The resultant stress distribution far from the surface predicted by this model (Equation 3.6) is much closer to the upper bound of the real surface cases at high loads. The average differences between the upper bound of the rough surface stress and both the Hertz and constant pressure stress predictions are summarized in Figure 3-11.



Figure 3-11: Average difference between the upper bound of the real surface stress distributions and those predicted by the Hertz contact model (solid line) and a constant pressure limit model (dashed line) as a function of load.

The upper bound stress can be predicted using simple models with average error less than 6 % if the correct model is chosen. For small loads, the stress corresponding to a Hertz pressure distribution should be used. For large loads, a constant pressure limit model is more accurate.

The transition from small to large load models can be approximated as the intersection of the two curves in Figure 3-11. In this case, the transition occurs at 535 N. Using Equation 3.13 with R=0.01 m (radius of the ball), the load at which plasticity is expected to occur (at 3 times the yield strength, 3Y) can be estimated as 359.87 N. However, this value corresponds to the onset of plasticity. Increasing the load will result in increased plastic deformation until the

plasticity spreads to the surface which is expected to occur at 6Y (Arnell et al. 1991). The load 535 N corresponds to a pressure that is *3.4Y*. This transition point can be used for the general case. Below this limit, the Hertz pressure model should be used. Above it, a constant pressure limit model is applicable.

## 3.3.4 Analysis Summary

The previous sections presented a simple model for near surface stress (constant pressure limit contact with radius  $a_s = (dx/2)\sqrt{2}$ ) and two models for stress far below the surface (Hertz pressure distribution or constant pressure limit contact with radius  $a_G = (3WR/4E^{*})^{\frac{1}{3}}$ ). The near surface stress model is valid from the surface to the location of the surface maximum at 0.48  $a_s$ . The model for global contact stress is valid below the location of the Hertz predicted maximum of 0.48  $a_G$ . The depths between the applicable locations for these models can be predicted using linear interpolation. This approximation is not exact, but its accuracy is not critical since these stresses will always be less than the maximum just below the surface and often less than the global maximum. Taken together, the approximations for near surface and global stress constitute a composite simple model for prediction of maximum subsurface stress.

The maximum stress distribution predicted by this simple model was compared to the upper bound of the maximum stress generated by a full numerical elastic-perfectly plastic simulation (Liu and Wang 2001) for a representative rough surface. Figure 3-12 illustrates the upper bound of the full numerical simulation and the maximum predicted by the surface and global stress simple models for applied loads of 100, 300, and 900 N.



Figure 3-12: Comparison of the upper bound of the real surface stress distribution to that predicted by surface and global stress simple models at 100, 300, and 900 N.

This comparison suggests that the simple models predict stress at the critical areas quite well. A more complete evaluation of the accuracy of this model will be presented in Part II which can be found in the next section of this chapter.

To summarize the simplified model, the following steps can be used to predict the maximum von Mises stress in elastic-perfectly plastic contact::

 Determine size of the smallest significant asperity (*dx*), operating conditions (*W*, *R*), and material properties (*E*', *v*, *P*<sub>lim</sub>).

- 2. Determine the location of the near surface maximum stress using  $a_s = (dx/2)\sqrt{2}$ and  $z_s^{\text{max}} = 0.48a_s$ .
- 3. Predict the maximum stress from the surface to the location of the near surface maximum,  $\sigma_{VM}(z = 0, ..., z_s^{\text{max}})$ , using Equation 3.6 where  $a = a_s$  and  $P_0 = P_{\text{lim}}$ .
- 4. Calculate the location of the global maximum stress using  $a_G = (3WR/4E')^{\frac{1}{3}}$ and  $z_G^{\text{max}} = 0.48a_G$ .
- 5. Calculate the limiting load using Equation 3.13 where *R* is the reduced radius and  $P_0 = 3.4Y = 3.4(P_{\text{lim}}/3)$ .
- 6. If the applied load is less than the limiting load, predict the maximum stress below the location of the Hertz maximum,  $\sigma_{VM} (z = z_G^{\max}, ..., \infty)$ , using Equation 3.14 where  $a = a_G$  and  $P_0 = P_{\lim}$ .
- 7. If the applied load is greater than the limiting load, predict the maximum stress below the location of the Hertz maximum,  $\sigma_{VM} (z = z_G^{\max}, ..., \infty)$ , using Equation 3.6 where  $a = a_G$  and  $P_0 = P_{\lim}$ .

This approach can be implemented as a computer program to execute the logical routines and mathematical functions. Such a program can be used to quickly and efficiently estimate maximum von Mises stress.

Analyses of subsurface stress are extremely important in engineering particularly for application specific surface design (Sayles 1996). As discussed in the Introduction, many excellent numerical methods for simulating elastic-perfectly plastic contact have been developed to address this need. However, in the engineering design process, it may not be practical to run time consuming contact simulations for every possible set of expected operating conditions and material properties. The simple model presented in this work provides an alternative method for quick estimation of the maximum von Mises stress.

## **3.4 Conclusions**

The subsurface stress field for elastic-perfectly-plastic contact between rough surfaces was analyzed. This analysis revealed trends that were validated by examination of the pressure and stress formulation. These trends were then used to develop an approximate model for prediction of the results of an elastic-perfectly plastic contact simulation. The location and magnitude of the maximum stress was found to be a function of the size of the smallest significant asperity, material properties, and operating conditions. This model can be used as a tool for quick estimation of the upper bound of the maximum stress distribution in rough surface contact.

## Chapter 4 Rapid Prediction of Maximum Stress, Part II

## 4.1 Background

In the previous chapter (Part I) a simplified model for rapid estimation of maximum subsurface stress was developed. Here, that model is further evaluated by comparison of the predicted maximum stress to that obtained using a full numerical solution. This comparison is made for contact with real rough surfaces, sinusoidal surfaces, ideal textured surfaces, and real rough surfaces with imposed computer generated texture. The magnitude of the difference between the upper bound predicted for a general surface by the simplified model and the maximum global contact stress for a specific rough surface is quantified. It is found that the degree of difference from the upper bound is directly related to surface roughness. The origin of the relationship between the global contact area. The enhanced simplified model enables rapid prediction of both the upper bound of the maximum subsurface stress for any surface and an estimate of the relationship between this upper bound and the expected maximum stress for a specific rough surface stress for any surface and an estimate of the relationship between this upper bound and the expected maximum stress for a specific rough surface. Some of the content of this chapter is also available in (Martini et al. In Publication).

## 4.2 Results and Analyses

## 4.2.1 Modeled System

The simplified model was evaluated for the system of dry, frictionless contact between an ideally smooth metallic ball and a rough metallic half-space. The material properties and operating conditions are the same as those described in (Martini et al. 2006) (R = 10 mm, E' = 110 GPA, v = 0.3,  $\sigma_Y = 678$  MPa, W = 200, 300, ..., 800 N). In the present work, the simplified model was evaluated using (a) real rough surfaces digitized using a white-light interferometer, (b) computer generated sinusoidal surfaces, (c) computer generated texturing imposed on ideally smooth surfaces, and (d) computer generated texturing imposed on digitized rough surfaces. These types of surfaces are described and illustrated in Table 4-1.

Туре	Sample	Roughness Description
Real Rough		Ground, honed, turned, and polished surfaces: Minimum $R_q = 0.15 \ \mu m$ Maximum $R_q = 1.07 \ \mu m$
Sinusoidal		$ \begin{array}{c} \overbrace{\lambda} \\ 1 < A < 5 \mu\text{m} \\ 35 < \lambda < 142 \mu\text{m} \end{array} $
Ideal Textured		$dx_{o}$ $dx_{o}$ $dx_{o}$ $dx_{o}$ $dx_{T}$
Real Rough Textured		$\int_{dx_{r}}^{dx_{o}} \int_{A}$ Same as Ideal Textured

Table 4-1: Types of surfaces used in the evaluation and enhancement of the simplifiedmodel for maximum stress prediction.

The digitized real machined surfaces were evaluated because direct digitization of real surfaces is thought to yield the most realistic description of surface characteristics (Liu et al. 1999). However, computer generated sinusoidal surfaces are also employed because they can be used as a means of controlling the surface characteristics and developing statistical relationships between the surface and contact properties (Johnson et al. 1985; Jaffar 1997; Gong and Komvopoulos 2003; Gao et al. 2006). Lastly, textured surfaces are introduced because surface texturing that has become increasingly popular as a means of improving component tribological performance (Etsion 2005; Pettersson and Jacobson; Zou et al. 2006) and therefore, the ability to predict changes in subsurface stress due to texturing is of significant interest.

### 4.2.2 Difference from the Maximum Stress Upper Bound

The accuracy of the simplified model is evaluated based on comparison to results obtained using a full numerical elastic-perfectly plastic simulation (Liu et al. 2000; Liu and Wang 2002). This model is chosen as a reference because perfect plasticity is a conservative approximation of plastic deformation that can be obtained with relative computational efficiency. The simplified model is intended to provide a rapid, conservative stress prediction. Therefore, the comparison to a perfectly plastic model is reasonable. To validate that the elastic-perfectly plastic model yields a more conservative result (i.e. higher maximum stress prediction) than an alternative, more complicated plasticity model, maximum stress predictions made by the two models were compared. Both simulations where run using the same operating conditions and material properties (those described in the previous section) and with a sinusoidal surface where  $\lambda = 120 \ \mu m$  and  $A = 3 \ \mu m$ . The plasticity model employed a linear hardening law in which the elastic plastic tangential modulus was 0.1 *E'*. A comparison of results revealed that the

maximum global contact stress predicted using the perfect plasticity assumption is greater than that predicted using the elastic-plastic solution. The difference between the two models is found to be larger at heavier applied loads. However, even at the smallest load considered, 100 N, the maximum global contact stress predicted with the perfect plasticity model is 1.6% larger. These comparisons support the statement that the perfect plasticity model yields a conservative estimation of maximum stress. Therefore, simulations based on the elastic-perfectly plastic model will be used going forward in this paper as a reference point to which the simplified model is compared.

The comparison between the simplified model and the full numerical solution will be focused on the locations of maximum stresses that are found near the surface due to asperity interaction and far from the surface due to the global shape of the contact. The focus is placed on these locations in component design because failure has been found to be initiated at stress concentrations (Kadiric et al. 2003). Therefore, the accuracy of the simplified model is considered the most critical at the points of maximum near surface and global contact stresses. These locations are illustrated for a representative real rough surface subject to applied loads of 200, 400, and 600 N ( $P_{Hz} = 2.5$ , 3.1, and 3.6  $\sigma_Y$ ) in Figure 4-1.



Figure 4-1: Distribution of the maximum stress (normalized by the material yield strength) at each depth below a typical rough surface for Hertz pressures of 2.5, 3.1, and 3.6  $\sigma_Y$ . Near surface (square) and global contact (circle) maximum stresses are identified.

A comparison between the maximum stress curves at these three applied loads indicates that the near surface stress maximum (represented by squares in the figure) is approximately constant. However, both the magnitude and depth of the global contact stress maximum (represented by circles in the figure) increases with load.

The simplified model was used to predict the maximum near surface and global contact stress for all surfaces described in Figure 4-1 and at applied loads from 200 to 800 N. The simplified model predicted maximum stresses were compared to results obtained using the full

numerical elastic-perfectly plastic simulation (Liu et al. 2000; Liu and Wang 2002). A comparison between the range of results obtained for the rough surfaces and the simplified model prediction is illustrated in Figure 4-2.


Figure 4-2: Magnitude of the near surface (top) and global contact (bottom) maximum stresses as functions of the Hertz pressure. Upper bound predicted by the simplified model represented by a solid line, the range of results for all rough surfaces evaluated by a shaded area, and the smooth surface result for global contact by stars. All values are normalized by the yield strength of the material.

It can be observed that the simplified model prediction of near surface maximum stress is good at all applied loads with an average error of 1.15% and a maximum error of 3.17%. In addition, the upper bound of the global contact maximum stress (i.e. the upper limit of the shaded grey area) is well captured.

The degree of difference between the global contact maximum stress upper bound predicted by the simplified model and the global contact maximum for a specific rough surface is found to be directly related to surface roughness, quantified by the root-mean-square ( $R_q$ ) measure of roughness, at all applied loads. That is, the upper bound of the shaded area in Figure 4-2 corresponds to surfaces with small  $R_q$  and the lower bound to surface with large  $R_q$ . This can be illustrated clearly using the results obtained for sinusoidal surfaces. Figure 4-3 shows the maximum global contact stress predicted by the simplified model and that calculated using the full numerical simulation for sinusoidal surfaces with a range of amplitudes and wavelengths.



Figure 4-3: Maximum global contact stress as a function of the Hertz contact pressure, both normalized by the material yield strength, for sinusoidal surfaces with amplitudes of 1 (squares), 3 (triangles), and 5 (circles)  $\mu m$  and wavelengths of 35 (solid symbols) and 142 (hollow symbols)  $\mu m$ . Smooth surface results indicated by stars and the upper bound predicted by the simplified model by a solid line.

This comparison reveals that the effect of sinusoidal wavelength is minimal. However, increasing amplitude corresponds to increasing overestimation of the simplified model. For sinusoidal surfaces, the  $R_q$  measure of roughness is linearly related to the amplitude (i.e.  $R_q = 0.5A$ ). Therefore, sinusoidal amplitude can be directly correlated to surface roughness and the relationship between  $R_q$  and the difference from the simplified model predicted upper bound is clearly illustrated.

#### 4.2.3 Enhancement of the Simplified Model

The analyses in the previous section revealed that the difference between the upper bound of the maximum global contact stress predicted by the simplified model and that maximum for a specific rough surface is directly related to surface roughness. By quantifying this relationship, the simplified model can be enhanced.

In the original simplified model, the upper bound of the maximum global contact stress is predicted using the original simplified model. The difference between the upper bound obtained using these steps and the maximum stress for a specific surface can be introduced as a correction factor, *C*, such that  $\sigma_G^{Max,Surface} = \sigma_G^{Max,UpperBound} - C$ . Based on the analyses of real rough, sinusoidal, and textured surfaces, this correction factor is expected to be a function of the surface roughness (quantified by the root-mean-square). In order to identify the form of this relationship, *C* is calculated for each rough, sinusoidal, and textured surface, as a function of surface roughness in Figure 4-4.



Figure 4-4: The difference between the simplified model predicted upper bound and the maximum global contact stress for a specific surface,  $C / \sigma_Y$ , as a function of the surface roughness,  $R_{q_2} / a_{H_z}$ . Different symbols correspond to different applied loads.

This figure shows that the correction factor increases with roughness and this relationship is approximately linear. In addition, the intercept of the line is zero. A zero intercept is expected since the difference from the upper bound decreases as the surface approaches ideally smooth (i.e.  $R_q=0$ ). A linear expression of the form  $(C/\sigma_Y) = m \times (R_q/a_{Hz})$  can be introduced. The data in figure 4 is used to obtain a best fit minimum value of m=45. The minimum slope is chosen in order to obtain the most conservative overall stress estimate. The error associated with this fit will be discussed later.

There is now a quantitative means of relating surface roughness to the difference between the simplified model-predicted upper bound and the maximum global contact stress for a specific surface. In order to implement this relationship as an enhancement to the simplified model, an additional step needs to be added to the end of the existing process.

New Step:

Estimate the global contact maximum stress for a specific surface by subtracting a factor

related to the surface roughness; 
$$\sigma_G^{Max,Surface} = \sigma_G^{Max,UpperBound} - m \left( \frac{R_q}{a_{Hz}} \right).$$

This new step was applied to the original simplified model and implemented to predict the maximum stress for all surfaces described in Figure 4-1. The effect of the enhancement is illustrated for a representative real rough surface in Figure 4-5.



Figure 4-5: Maximum global contact stress for a real rough surface with  $R_q = 0.28 \ \mu m$  predicted by the original simplified model (solid line), the simplified model with the enhancement introduced in this paper (solid line with stars), and a full numerical elastic-perfectly plastic solution (broken line).

This figure illustrates that the difference between the simplified model prediction and the full numerical solution for this surface is decreased by use of the enhancement. This behavior was observed for all surfaces and applied loads. The average and maximum percent differences between the maximum global contact stress predicted using the enhanced simplified model and that obtained using the full numerical elastic-perfectly plastic solution are illustrated in Figure 4-6.



Figure 4-6: The average (solid shapes) and maximum (hollow shapes) percent difference between the original (stars) and the enhanced (trapezoids) simplified model and the full numerical solution result for all surfaces evaluated as function of load.

It is clear from this image that both the average and maximum differences are reduced by introduction of the enhancement. In fact, the degree of this reduction for a specific surface is typically found to be on the order of 3 times.

# 4.3 Discussion

It was observed that the difference between the upper bound predicted by the simplified model and the maximum global contact stress for a specific surface is a function of the roughness of that surface. Physically, this indicates that a rougher surface lowers the global contact stress. This is an interesting finding as roughness is typically thought to have a significant effect only on the near surface stress distribution. The origin of the relationship between roughness and global contact stress can be investigated in terms of the size of the apparent contact area, which is quantified by the radius of the circle inscribing the outer most contact areas. It should be emphasized that this discussion is in reference only to the apparent contact area, not the actual contact area on which surface roughness may have a very different effect.

It was observed from the simulation results that the global contact stress decreases with increasing surface roughness. Global contact stress is inversely related to contact area. Therefore, the relationship between global contact stress and surface roughness can be understood if surface roughness increases the apparent contact area. This possibility can be evaluated directly using the surface separation distributions predicted using the full numerical elastic-perfectly plastic simulation. Consider a set of ideally smooth textured surfaces with roughness amplitudes ranging from 0 (no texture) to 5  $\mu$ m. The deformed surface profile along the contact centerline and a close of that profile at the perimeter of the apparent contact aarea for a representative load is illustrated in Figure 4-7.



Figure 4-7: Deformed surface profile for  $P_{Hz}$ =3.6  $\sigma_Y$  along the contact centerline (top) and close up of that profile at the perimeter of the apparent contact area (bottom) for texture depths of 5 µm, 3 µm, 1 µm, and no texture (from left to right).

The location of the edge of the surface profile corresponds directly to the size of the apparent contact area. That is, as the surface profile in the lower image moves left, the apparent contact area increases. Figure 4-7 illustrates that when deformed, the surface with no texturing (profile

to the far right) has the smallest apparent contact area, and that the size of the apparent contact area increases with increasing texture depth. This relationship between surface roughness and apparent contact area provides the link between global contact stress and surface roughness. Increasing roughness results in larger apparent contact area which in turn corresponds to a smaller maximum global contact stress.

#### 4.4 Conclusions

An enhancement to a simplified model for prediction of subsurface stress was developed which introduces the effect of surface roughness on the magnitude of the maximum global contact stress. It was found that increasing surface roughness corresponds to a larger difference between the simplified model-predicted upper bound for any surface and the maximum stress for a specific rough surface. This relationship was quantified using simulation data obtained for a variety of digitized real and computer generated surfaces. An empirical expression was fit to the data in order to add a new step to the simplified model. The relationship between surface roughness and maximum global contact stress was explained in terms of apparent contact area. The developed enhancement expands the functionality of the simplified model which may enable improved performance and wear prediction in component design.

# Chapter 5 Evaluation of a Mixed EHL Wear Model

# 5.1 Background

In this last chapter on continuum modeling, the topic of wear in mixed elastohydrodynamic lubricated interfaces is introduced. Sliding wear is a significant surface failure mode in many mechanical components. The magnitude of changes in surface topography due to wear may be comparable to or larger than the original surface roughness and elastic deformation (Goryachev 1998). In addition, wear induced changes in the size and shape of the contact area may alter the direction and magnitude of forces that act on the surface (Sugimura and Kimura 1984). As a consequence, machine component functionality may be affected. However, these effects have rarely been incorporated into numerical simulation models used as predictive tools in engineering practice. There are two primary difficulties that have been obstacles in the wear simulation research. First, the amount of wear is directly related to local lubrication effectiveness and contact severity, which are difficult to quantify in mixed lubrication, especially when a full-scale deterministic model is not available. Smooth surface assumption and stochastic surface models may not be satisfactory for the prediction of local contact severity and application of material failure criteria. A good model needs to incorporate the effects of hydrodynamic flow, elastic deformation of the contacting bodies, surface roughness and topography, as well as possible change of viscosity and density with pressure. Simple models with one or two stochastic parameters may not be sufficient to describe these integrated and complicated phenomena. The second difficulty is the mutual dependency of wear

and mixed lubrication characteristics. Wear changes the surface topography in real time. The surface topography may, in turn, significantly affect mixed lubrication characteristics and the contact severity. Contact severity may then greatly influence the wear process immediately. This interdependency is difficult to describe with simplified time-independent models, and satisfactory solution may require a transient deterministic simulation.

Wear takes place at locations where surfaces are in direct contact. The amount of material removal is directly correlated to "contact severity", which is a complicated concept that may involve contact pressure, sliding speed, asperity deformation, interfacial temperature, friction, subsurface stresses and some other parameters. Depending on the problem, contact severity may need to be described in different ways. As a result, different forms of wear equation may be obtained. Meng and Ludema (Meng and Ludema 1995) reviewed thirty-five years of the journal Wear and fourteen years of proceedings from the Wear of Materials conferences, and 182 distinct wear equations were reported. However, in a detailed analysis of these models, including their development method, regime of applicability, variables, and experimental verification, it was concluded in (Meng and Ludema 1995) that none was sufficient to described complicated wear phenomenon in general. More strikingly it was concluded that future (improved) wear models are not likely to be obtained from synthesis of existing equations or even using approaches taken in the past. Based on these viewpoints, it was proposed that a successful approach to wear modeling must incorporate "full description of the evolution of macroscopic events on sliding surfaces" (Meng and Ludema 1995).

Recently, deterministic mixed lubrication models have been developed (such as those presented by Zhu and Hu et. al. in (Hu and Zhu 2000; Zhu and Hu 2001; Zhu and Hu 2001)),

which solve both hydrodynamic lubrication and surface contact simultaneously, and predict the distributions of pressure, film thickness, asperity deformation, subsurface stresses, friction and interfacial temperature, etc. as functions of location and time. Also, the deterministic simulation is based on real measured digitized surface topography, so that arguments on selection and application of stochastic parameters can be avoided. This enables application of a more sophisticated approach that provides a full numerical transient mixed lubrication model, capable of predicting contact severity at local spots, and the ability to handle the mutual dependency between wear and mixed lubrication characteristics. Such a model was developed and implemented as a simulation tool.

The contribution to this work described here is an evaluation of the mixed EHL wear model by comparison of simulation predicted trends with experimental observations from the literature. Three different EHL simulation cases are considered and analyzed in terms of predicted surface topography evolution, properties of the lubricated interface, and the phases of wear. Results show basic trends in good agreement with experimental observations and indicate that this numerical approach can be used to simulate surface topography evolution due to sliding wear. Some of the content of this chapter is also available in (Zhu et al. Accepted).

#### 5.2 Model Summary

#### 5.2.1 Wear Modeling Background

The available deterministic mixed lubrication model can predict contact and lubrication characteristics, such as distributions of contact pressure, lubricant film thickness, and so on. However, before simulating material removal due to wear at each contact spot, a correlation between the mixed lubrication characteristics and the local material removal needs to be established. It is understood that wear characteristics may be functions of various material properties and operating conditions as well as consequent local physical parameters. Many different theoretical and empirical models have been developed in previous studies to define this relationship for different applications. In one review article, it was found that 32 different parameters were used by various wear law authors to describe their data (Hsu et al. 1997). In another, over 100 unique variables and constants were identified (Meng and Ludema 1995). This inconsistency has primarily been caused by a lack of powerful analysis tools such that researchers have had to employ many different simplifications under different conditions. Inconsistency is also caused by varying understandings of how to define and describe contact severity and its resultant wear in different applications. However, upon reviewing a large number of previously developed wear models (see (Meng and Ludema 1995; Hsu et al. 1997; Goryachev 1998)) it is believed that the most common of these expressions can be put in the form of a single equation, in which wear rate, dW/dt, is a function of contact pressure, p, relative sliding velocity, u, and material hardness, H.

$$\frac{dW}{dt} = k \frac{p^{\alpha} u^{\beta}}{H^{\gamma}}$$
(5.1)

In Equation 5.1, *k* is the wear coefficient and the three exponential constants,  $\alpha$ ,  $\beta$ , and  $\gamma$ , differ based on which wear law is being used. Table 5-1 summarizes the value of these exponents for some representative wear laws among the many previously published theoretical and empirical wear laws.

Table 5-1: Summary of some empirical and theoretical wear laws with corresponding exponential constants for pressure (load in the case of empirical expressions),  $\alpha$ , sliding velocity,  $\beta$ , and hardness,  $\gamma$ . Wear models obtained from (Goryachev 1998) unless otherwise specified.

	α	ß	γ	Additional Terms	Primary Application	
Empirical:						
Lewis(1968)	1	1	0		Adhesion of filled PTFE and piston rings	
Khrushchov and Babichek (1970)	1	1	1		Micro-cutting of metals	
Rhee (1970)	α	β	0	Exponential function of t	Adhesion with thermal effects	
Lancaster (1973)	1	1	0	Includes wear rate correction factors	Filled thermoplastics and filled PTFE	
Larsen-Basse (1973)	1	1	0	Defined in terms of impact frequency	Thermal fatigue and carbide polishing	
Moor, Walker and Appl (1978)	1	1.8	0	<i>p=p</i> (rock volume removed / distance)	Wear of diamond inserts and rotary drag bits	
Luo, et.al. (2005), (Luo et al. 2005)	0	1	1	Normal stress between tool flank face and work piece	Adhesion/abrasion of cutting tool flank	
Cayer-Barrioz et.al. (2006), (Cayer- Barrioz et al. 2006)	2	1	0	Molecular weight	Abrasion of polymeric fibers	
Theoretical:						
Holm (1946)	1	1	1		Adhesion	
Archard (1953)	1	1	1		Adhesion	
Kragelsky (1965)	>1	1	0		Fatigue	
Rabinowicz (1971)	1	1	1		Abrasion / Fretting	
Harricks (1976)	1	1	0		Fretting	

The wear coefficient differs based on the material properties and operating conditions to which each wear law is applicable. For the cases evaluated here, Archard's wear law, where  $\alpha = \beta = \gamma = 1$ ,

will be employed. Archard's model is frequently referenced because of its simplicity and wide application in different practical cases (Hsu et al. 1997; Bajpai et al. 2004).

### 5.2.2 Mixed EHL Simulation Overview

The simulation used in this work can be considered to be an enhancement of the existing mixed-EHL model (Hu and Zhu 2000; Zhu and Hu 2001; Zhu and Hu 2001). The original model incorporated the effects of hydrodynamic flow, elasticity, and lubricant behavior. The hydrodynamic effects are governed by the Reynolds equation. Elasticity of the contacting solids is modeled based on deformation due to normal pressure distribution. Mixed lubrication friction is considered to be the sum of hydrodynamic friction and contact friction. The hydrodynamic friction is calculated in hydrodynamically lubricated areas using Bair and Winer's non-Newtonian elastic-viscous fluid model. Friction in the contact areas is obtained using an experimentally estimated boundary lubrication coefficient of friction (typically between 0.08 and 0.12). Changes in viscosity and density with pressure are modeled by the Barus equation and the Dowson-Higginson, equation respectively (Hu and Zhu 2000; Zhu and Hu 2001; Zhu and Hu 2001). The surface deformation and subsurface stresses are calculated from the contact pressure and friction using the discrete convolution and fast Fourier transform (DC-FFT) approach developed by Liu and Wang (see (Liu et al. 2000; Liu and Wang 2002) for details), so that the computational speed is greatly increased.

Wear is integrated into the model as an additional term in the expression for instantaneous film thickness (or gap between the surfaces). With this addition, film thickness, *h*, is the sum of the geometry of the contacting bodies ( $B_x$  and  $B_y$ ), roughness of the surfaces ( $\delta_1$  and  $\delta_2$ ), elastic deformation (*V*), and surface changes due to wear ( $W_1$  and  $W_2$ ). The wear of the two surfaces

must be introduced separately because their material properties may differ resulting in different wear behavior.

$$h = h_0(t) + B_x x^2 + B_y y^2 + \delta_1(x, y, t) + \delta_2(x, y, t) + V(x, y, t) + W_1(x, y, t) + W_2(x, y, t)$$
(5.2)

As described in the previous section, the wear on a given surface is a function of the wear coefficient, pressure, sliding velocity, and material hardness. Assuming that the wear coefficient, sliding velocity, and hardness are independent of time and surface location, the following expression arises:

$$W(x, y, t) = k \frac{u^{\beta}}{H^{\gamma}} \int p_c^{\alpha}(x, y, t') dt'$$
(5.3)

With this approach, the model can be easily modified for application to different material properties or operating conditions by adjusting the coefficients in Equation 5.1 per the appropriate wear law. In addition, it is feasible that any mathematically expressed wear law (even one not in this form) could be integrated into the simulation with relative ease.

#### **5.2.3 Simulation Parameters**

Simulations of three different mixed EHL cases were performed. The first is a contact between an ideally smooth surfaced sphere sliding across a stationary flat surface with computer generated sinusoidal roughness. The next is a contact between a sphere and a flat where both surfaces are ground and both are moving. And lastly, a simulation of a ball-on-disk bench test experiment. The ball-on-disk case was chosen such that the wear coefficient used in the simulation can be calibrated using comparable experimental data. The operating conditions and material properties for these three cases are summarized in Table 5-2. Table 5-2: Summary of operating conditions and material properties for the three mixed-EHL simulation cases performed.

Case Name:	Sinusoidal	Ground	Ball-on-Disk
Description	Smooth sphere on sinusoidal flat	Ground sphere on ground flat	Ball-on-disk test specimens
Operating Conditions:			
Applied Normal Load (N)	800	1600	444
Radius of Curvature (mm)	19.05	19.05	5.35
Ball Surface Velocity (m/s)	0.1	3.75	0
Flat Surface Velocity (m/s)	0	5.25	0.798
Solid Properties:			
Young's Modulus (Gpa)	200	200	206
Poisson's Ratio ()	0.3	0.3	0.3
Density (g/cm^3)	7.865	7.865	7.865
Hardness (Gpa)	3	2.5	7.5
Yield Limit (GPA)	0.5	0.5	0.5
Wear Coefficient ()	0.0045	0.005	0.002
Surface Properties:			
Ball RMS Roughness (micron)	0	1.14	0.025
Flat RMS Roughness (micron)	0.8	1.155	0.3
<b></b>			
Lubricant Properties:			
Viscosity (Pa.s)	0.096	0.096	0.01119
Pressure-Viscosity Coeff. (1/Gpa)	18.2	18.2	14.94
Density (g/cm^3)	0.88	0.88	0.866

In each of these cases, the simulation was initialized with simulation of ideally smooth surfaces. Then, the digitized rough surfaces were incorporated and the simulation run with no wear for approximately 500 cycles, which was sufficient for numerical stabilization. Lastly, the effect of wear was added and the simulation continued for at least 3000 more cycles. After each cycle, contact parameters were saved to data files for analysis later.

# 5.3 Results and Analyses

# 5.3.1 Surface Evolution

One analysis that can be performed using the transient solution generated by the present wear model is that of surface evolution over time. This is an important investigation because the evolution of surface topography is readily captured using experimental techniques and therefore may be used for model validation. The evolution of the two surfaces predicted by the ball-ondisk simulation is shown in Figure 5-1.



Figure 5-1: Evolution of the disk wear track (left) and ball wear scar (right) over time. Ball image length scale is larger than that of the disk to facilitate visual analysis. Snapshots of the surfaces are shown without wear and at 1000, 2000, and 3000 cycles after the wear process begins.

There is no visible wear track on the disk, or scar on the ball before wear is introduced. Then, the contrast between the worn and unworn areas on the surfaces increases. Both the ball and disk exhibit characteristic wear patterns typically observed in experimental studies of lubricated sliding contact. The worn disk surface contains a track with texturing parallel to the direction of sliding. And the ball surface is worn first at the contact inlet. Both of these trends agree with experimental observations (Sugimura and Kimura 1984; Kuo et al. 1996).

A similar surface evolution analysis was performed for the ground surface simulation. Snapshots of the two surfaces as they change over time are shown in Figure 5-2.



Figure 5-2: Evolution of the two ground surfaces moving at 3.75 m/s (left images) and 5.25 m/s (right image). Snapshots of the surfaces are shown without wear, and at 1000 and 2000 cycles after the onset of wear.

The evolution of the ground surfaces exhibits the expected trends of not only increasing wear with time, but also the effect of surface velocity on wear rate. The wear model employed (given in Equation 5.1) defines wear rate in direct proportionality to surface velocity. Consistent with this definition, more wear is visible on the faster moving ground surface (right images in Figure

5-2). These qualitative comparisons of surface evolution from the ball-on-disk and ground surface simulations provide partial validation of the present model. In addition, the surface detail files generated by the simulation after each cycle make possible a variety of quantitative comparisons.

# 5.3.2 Contact Properties Before and After Wear

EHL simulations are frequently used to predict film thickness and pressure distributions in the contact area. Therefore, it is of interest to analyze these parameters before and after wear is incorporated into the simulation. Film thickness is represented by a contour plot where regions of dimensionless film thickness (normalized by the Hertz contact radius) less than 0.000002 (corresponding to small dimensional values less than 0.53-0.94 nm depending on the simulation case) are in white. Contact pressure is represented by a contour plot in which regions where the dimensionless pressure (normalized by Hertz pressure) greater than 1.3 are in white. For the sinusoidal surface case, this comparison is illustrated in Figure 5-3.



Figure 5-3: Film thickness (top) and pressure (bottom) distributions for the sinusoidal surface contact case simulated with (right) and without (left) wear.

Comparison of these images reveals two significant differences between the contact behavior before and after wear. First, the overall contact area is larger in the case with wear after 3000 cycles. And second, the sinusoidal asperity peaks are reduced resulting in a more uniform overall appearance of the contact pressure and film thickness distributions.

The trends observed in the sinusoidal case were also found in simulation of ground surface contact. The contact pressure and film thickness distributions for the ground case are shown in Figure 5-4.



Figure 5-4: Film thickness (top) and pressure (bottom) distributions for the ground surface contact case simulated with (right) and without (left) wear.

The ground surface film thickness and pressure distributions exhibit the same trends of larger contact area and increased uniformity as were observed with the sinusoidal case. In addition, the effect of an established wear track in each case is also to change the shape of the contact area from circular to elliptical. This phenomenon is described graphically by the simplified contact illustrations in Figure 5-5.



Figure 5-5: Illustration of the shape change of the contact zone due to an established wear track.

The effect of wear can also be identified through analysis of subsurface stress. The pre and post wear stress distributions for the ground case (shown with the centerline film thickness and pressure for clarity) are illustrated in Figure 5-6.



Figure 5-6: Centerline subsurface stress distribution with (right) and without (left) wear for the ground surface contact case. Dimensionless centerline pressure and film thickness shown above the stress distribution for clarity.

Analysis of the ground surface stress distributions reveals that the changes in the contact area due to wear have a significant effect on subsurface stress. The large stresses just below the surface (caused by severe contact between asperity peaks) move closer to the surface due to the reduction of asperity size with wear. As larger asperity peaks are removed, the smaller, high frequency asperities become more prevalent. This results in an increase in frequency of the corresponding near surface stress peaks. Wear also affects the stress further below the surface due to the change of the contact shape and the corresponding redistribution of the overall stress field. The effects that wear-induced contact area changes have on stress are particularly critical as they have been found to accelerate failure modes in addition to material loss (Bajpai et al. 2004).

Pre and post wear analyses were also performed for the ball-on-disk case. The film thickness and pressure distributions for this simulation case are illustrated in Figure 5-7.



Figure 5-7: Film thickness (top) and pressure (bottom) distributions for the ball-on-disk contact case simulated with (right) and without (left) wear.

The ball-on-disk contact simulation exhibits the same trends of contact area expansion and increased uniformity as were observed in the sinusoidal and ground cases. However, the shape of the contact area does not appear to change as much as it did the ground case. The ball-on-disk case exhibited one feature not observed in the ground case where the center of the contact area in the direction of sliding was more affected by the wear than the outer edges. This is due to the fact that only one of the surfaces is moving in the ball-on-disk case whereas both are moving in the

ground contact. The effect of wear on subsurface stress for the ball-on-disk case was analyzed as illustrated in Figure 5-8.



Figure 5-8: Centerline subsurface stress distribution with (right) and without (left) wear for the ball-on-disk case. Dimensionless centerline pressure and film thickness shown above the stress distribution for clarity.

The subsurface stress in the ball-on-disk case underwent redistribution due to wear similar to that observed with the ground surfaces. The near surface stress peaks moved closer to the surface and increased in frequency while the global contact stress decreased. In addition, wear causes the location of the global contact stress to move further from the surface. This is a direct result of the increased overall contact area.

# 5.3.3 Phases of Wear

A typical system may be subject to wear in three phases: initial running-in, relatively steady state, and accelerated or catastrophic wear. The running-in phase occurs in the beginning and is associated with a high wear rate. During the running-in phase, tall asperity peaks are quickly removed and the surfaces become smoother. After the tallest peaks are removed, the wear rate decreases and gradually stabilizes. In the steady-state stage, the wear rate is relatively stable, and it is in this phase that it is desirable for machine components to operate as long as possible. Lastly, in some cases, steady-state gives way to catastrophic wear in which the wear rate once again increases (Goryachev 1998; Yuan et al. 2005; Nelias et al. 2006). This is only a general description of the overall wear process, and specific cases differ from one to another. In some cases, for example, the running-in may be too short to observe, while in other cases, a system may not undergo catastrophic wear even after a very long time.

The expected phases of wear were evaluated using the present simulation by analysis of the change in wear volume removed from the surface over time. This analysis is illustrated in Figure 5-9.



Figure 5-9: Wear volume as a function of time for the three contact simulation cases analyzed. Inset shows a close-up of trends observed at the onset of wear.

The first 500 cycles of the simulation are run without wear. During this phase, as expected, there is no wear volume generated. Then, wear is introduced to the simulation. A close up view of the immediate response is illustrated in the inset of Figure 5-9. It can be seen from this image that there is a brief running-in period where the wear increases rapidly for all three cases. However, this increase is found to be most significant in the sinusoidal surface case and least significant in the ground surface case. These results are consistent with experimental observations of the running-in phase. Both rapid wear increase and variation of the intensity of this increase with

different operating conditions have been reported by other researchers (Sugimura and Kimura 1984).

After running-in, the wear enters the steady state phase where the wear rate is relatively constant (i.e. constant wear-time curve slope). This phase appears to last quite long. The wear rate during the steady state phase is different for the three contact cases evaluated. As can be seen from the slope of the curves in Figure 5-9, the ground surface wear rate is higher than the other two. This is consistent with experimental observations that fractional contact area increases due to wear most significantly on surfaces with transverse roughness (Lo and Tsai 2004) such as the ground surfaces evaluated here. After this phase of relatively steady wear, the wear rate appears to gradually increase again indicating a transition to accelerated or catastrophic wear.

The phases of wear that a system goes through can, in some cases, be correlated to the change in the friction coefficient over time (Yuan et al. 2005). The friction coefficients for each case calculated by the present simulation are given in Figure 5-10.



Figure 5-10: Friction coefficients as a function of time after the introduction of wear (plots start at 500 cycles) for each simulated contact case.

In all three cases it is assumed that the contact friction coefficient is 0.1, which provides an upper limit of possible friction variation. It is observed that at the beginning where there is no wear yet, the friction coefficient is quite high, close to 0.1, due to severe asperity peak contacts. Then, there is a sharp decrease of the friction coefficient immediately after wear is introduced into the simulation. This corresponds to the running-in phase in which tall asperity peaks are worn away quickly and the surface undergoes mechanical polishing. After this initial drop off, the friction gradually goes up. This is consistent with similar trends observed experimentally in both dry and lubricated contacts. In analysis of experimental results, the increase of friction with sliding distance has been directly related to measured values of both real (Lo and Tsai 2004) and apparent contact area (Kuo et al. 1996).

The direct relationship between friction and contact can be seen through the correlation between the friction coefficient and the contact load ratio. This relationship is illustrated in Figure 5-11 for the ball-on-disk case.



Figure 5-11: Friction coefficient (solid line) and contact load ratio (hollow squares) as functions of time for the ball-on-disk case illustrating the relationship between friction and contact area during the wear process.

The sharp decrease in friction observed during the running-in phase is consistent with a sharp decrease in the contact load ratio from approximately 0.7 to 0.3. Physically, this corresponds to a

decrease in the percent of the load supported by contact locations (i.e. decreasing overall contact area). Then, the subsequent gradual increase in friction is concurrent with an increase in the contact load ratio. Here, the contact area is getting larger and the friction is increasing correspondingly. The other cases evaluated exhibited similar consistency between the contact load ratio and the friction coefficient.

#### **5.4 Conclusions**

A model for wear in mixed-EHL was evaluated to determine whether wear behavior predicted by the simulation correlate with experimentally observed trends. The simulated wear process exhibited a running-in phase, followed by stabilization and possible acceleration, which is consistent with test data. Predicted wear was found to be correlated with variations of material hardness, sliding speed, applied load and wear coefficient as expected based on the implemented wear model. And surface evolution and wear track establishment predicted by the simulation appeared reasonable and agree qualitatively with experimental observations. Therefore, it is likely that the developed simulation will provide a powerful tool for wear modeling and failure prediction in component design.
# **Chapter 6**

## Molecular Model of Thin Film Lubrication

#### 6.1 Background

This chapter begins the transition of the dissertation from primarily continuum-based studies to molecular-scale analyses. The first step in this transition is development of the necessary simulation tools. Development was based on an existing molecular simulation tool, *MU*/tipurpose *SI*mulation *Code* (MUSIC) (Gupta et al. 2003), which was originally designed to model flexible sorbate molecules in zeolites. Enhancements were made to that code to introduce the important characteristics of a thin film lubricated interface. These characteristics include appropriate interaction models for the lubricant molecules and walls, imposing shear on the fluid via wall movement, temperature control during the simulation which allows fluid heating, and identification of an appropriate confined fluid density. The resultant simulation not only is representative of a thin film lubricated interface, but allows investigation of the unique properties of thin film such as their density, solvation pressure, interface slip, and viscosity. The simulation description in this chapter is also summarized in (Martini et al. 2006) and (Lichter et al. Accepted).

#### 6.2 Model Overview

In general, MD simulations model molecules and their interactions by potential energy functions. Forces are obtained by analytical differentiation of these potentials. Positions and velocities are then calculated by numerical integration of the resulting equations of motion. The integration of the equations of motion is performed using a 6<sup>th</sup> order Gear predictorcorrector algorithm. This method involves three steps: prediction, evaluation, and correction. First, the new positions and their derivatives are predicted using a fifth-order Taylor series expansion based on current positions and derivatives. Next, the forces on each atom are evaluated based on the predicted positions. Lastly, the predicted positions and derivatives are corrected based on the difference between the predicted acceleration and that from the force evaluation (Haile 1992).

The time step for a molecular dynamics simulation must be chosen such that it is small enough to prevent instabilities in the integration algorithm and large enough that the phase space is covered efficiently. The general rule is that the time step should be at least one order of magnitude smaller than the shortest period of motion (Leach 2001). For the model used in this research, the natural time scale of motion due to the spring potential, Lennard-Jones interactions, bond bending and bond torsion must be considered. The time scale of the wall spring oscillation is a function of the spring constant and the mass as given in Equation.6.1.

$$t_{spring,0} = \sqrt{\frac{m}{k}} \approx 1.2\,ps \tag{6.1}$$

The time scale of the Lennard-Jones interactions is a function of the Lennard-Jones energy and distance parameters as given in Equation 2.2 (Liem et al. 1992).

$$t_{LJ,0} = \sqrt{\frac{m\sigma^2}{\varepsilon}} \approx 1.7 \, ps \tag{6.2}$$

The time scale of the bond bending and torsion are significantly smaller than both of these. It is suggested by Leach that an appropriate time step size for flexible molecules subject to translation, bond bending, and bond torsion is 0.002 ps (Leach 2001). However, to ensure stability, a time step of 0.001 ps was used in this research. This value was selected because it was used successfully with the MUSIC simulation tool previously.

All simulations were run in the ensemble of constant number of particles, volume, and temperature (NVT). Periodic boundary conditions were applied in the directions in the plane of the walls (X and Y). A snapshot of a typical simulation cell at a single time step is illustrated in Figure 6-1.



Figure 6-1: Snapshot of the simulation cell illustrating the coordinate axes, a typical configuration of the walls and fluid, and the direction of the constant wall velocity imposing shear on the fluid.

#### 6.3 Simulation Details

#### 6.3.1 Imposing Shear

To simulate thin film lubrication, the modeled fluid must be sheared. In this research, a boundary-driven method is employed in which shear is imposed on the fluid by simulating wall-fluid atom interaction and then moving the wall atoms (Khare et al. 1996). This approach was chosen because it is considered to be closely analogous to the physical system being simulated (Liem et al. 1992). In addition, it enables temperature to be controlled without adjusting the velocities of the fluid atoms as is discussed in the next section. The wall movement is implemented by moving each atom in the walls through a distance equal to a predefined velocity multiplied by the time step. The wall atoms are moved after the correction step in the Gear integration algorithm.

#### 6.3.2 Temperature Control

In a shear flow simulation, the work that is done on the system in the form of the shearing is converted to heat in the lubricant. Therefore, in order to maintain constant temperature, it is necessary to remove the heat from the system using a thermostat. Researchers have used a variety of approaches to do this including thermostatting all the atoms in the system (lubricant and wall) (Hu et al. 1996), all fluid atoms in the non-shear directional components (Zhang et al. 2001), all the wall atoms (Liem et al. 1992; Khare et al. 1996), thin layers of fluid atoms near the walls (Balasundaram et al. 1999), and atoms in the outer layers of the walls (Tanaka et al. 2003). In the latter three cases in which all or most of the lubricant atoms are not thermostatted, it has been found that there is significant viscous heating in the lubricant. This is desirable as it is

consistent with experimental observations (Balasundaram et al. 1999). It is important to allow the simulated fluid to undergo this temperature increase because it may have significant effect on lubricant rheology (Stachowiak and Batchelor 2001).

For the model verification system, the temperature of the system will be controlled by thermostatting all of the atoms in the walls such that the temperature of the walls is maintained at 300 K. This method was chosen because it is analogous to the experimentally observed conduction of frictional heat out of the fluid through the solid walls (Cui et al. 1999). In the analogous macroscopic case, frictional heat is transmitted from fluid to walls via both conduction and convection. However, it has been shown that the primary mechanism in thin film lubrication is conduction (Stachowiak and Batchelor 2001). Frictional heating will be simulated in MD by allowing the fluid to heat up. This heat is then transferred to the walls by molecular interaction and removed from the walls by the thermostat. It has been suggested that thermostatting only the outer wall layers (Tanaka et al. 2003). However, this method is inefficient because it requires longer simulation time to obtain steady state. Since thermostatting only the outer wall layers has not been proven to have a positive impact, it was not implemented in this research for computational efficiency reasons.

The temperature control method used for this work is the Nose-Hoover thermostat. In this method, an additional degree of freedom is added to the system to represent contact with a thermal reservoir. Energy is then transferred between this extended system and the rest of the simulation. This is accomplished by relating the extra degree of freedom, *s*, to the atomic velocities according to  $v = s\dot{r} = p/ms$ . The new equations of motion for the system then

become those given in Equation 6.3 where Q is the thermal inertia parameter and *dof* is the number of degrees of freedom (Arnell et al. 1991).

$$\ddot{r} = dof / ms^2 - 2\dot{s}\dot{r} / s$$

$$Q\ddot{s} = \sum_i m\dot{r}_i^2 s - (dof + 1)k_B T / s$$
(6.3)

The thermal inertia parameter controls the rate of energy transfer. As will be discussed in the next section, energy transfer is also affected by the wall spring constant. In this research, it was found that the effect of using different values of Q between 1 and 1000 ps<sup>2</sup> kcal/mol was minimal. Therefore, Q=100 ps<sup>2</sup> kcal/mol was selected, as that value has been used in past applications of the MUSIC simulation code.

#### 6.3.3 The Wall Model

The wall atoms are initially arranged in a face-centered cubic (FCC) lattice. This arrangement was chosen because it is commonly used in the literature and therefore convenient for results comparison. In addition, it is one of the structures into which most homogeneous metals crystallize. The FCC unit cell arises from the cubic close-packed atomic stacking pattern which can be explained in terms of organizing atoms into the closest possible packing (Atkins 1978). A single FCC unit cell is illustrated in Figure 6-2.



Figure 6-2: Face-centered cubic unit cell arrangement for the initial wall atom configuration.

The atomic spacing within the unit cell must be chosen such that the fluid atoms do not penetrate the walls (Khare et al. 1996). This limitation can be expressed as a relationship between the Lennard-Jones distance parameter,  $\sigma$ , and the nearest neighbor distance, d. For the solid noble gases, this relationship is  $d \approx 1.09\sigma$  (Cui et al. 2001). From the nearest neighbor distance, the size of the FCC unit cell can be calculated. A single unit cell is then created which can be copied in each of the three directions to create a wall of the desired size. For most of the simulations run in this research, the length of each wall in the X (shear) and Y directions is 32 Å. There are two layers of unit cells in the Z direction in each wall. The total number of atoms in each wall is 512.

The wall atoms are prevented from "melting" by use of a restoring spring potential that tethers the wall atoms to their face centered cubic lattice sites. This method of maintaining solidity of the walls during the simulation is commonly used (Liem et al. 1992; Jabbarzadeh et al. 1998). The potential energy function has the form  $\Phi_{spring} = \frac{1}{2}k(r - r_{lattice})^2$  where k is the spring constant.

The wall lattice structure serves the purpose of both providing structure to the wall boundaries and acting as a heat sink for the frictional heat generated due to the shear (Liem et al. 1992). The value of the spring constant, k, is an important parameter because it affects both the fluid-to-wall energy transfer rate and the solidity of the walls (Cui et al. 1999). It must be small enough that the thermal motion of the wall atoms can efficiently transfer frictional heat out of the fluid. However, it must also be large enough that the walls remain solid.

There is no definite guideline for choosing the value of k. However, a method has been suggested in which the spring constant is a function of the Lennard-Jones energy and distance parameters for the wall-wall interactions,  $k = (72\varepsilon_{ww}/2^{1/3}\sigma_{ww}^2)$  (Liem et al. 1992). For the simulations described here, this criterion was used only as a guideline for selecting the value of the spring constant. The Lindemann criterion for melting can also be used to quantify wall solidity. This expression is  $\langle \delta u^2 \rangle / d^2 \leq 0.023$  where d is the nearest neighbor distance and  $\langle \delta u^2 \rangle$  is the mean squared displacement around the lattice sites (Thompson and Troian 1997).

The approach taken in this research was to identify favorable values of k by trial and error, and then ensure that the Lindemann criterion was satisfied. The affect of the spring constant on both the solidity of the wall and the heat transfer from the fluid to walls were considered in this evaluation.

First consider the solidity of the wall. To illustrate this effect, consider Figure 6-3 which shows snapshots of the atomic configuration for two different values of k.



Figure 6-3: Configuration of fluid (grey) and wall (orange) atoms after 250 ps for (a) k=1 amu/ps<sup>2</sup> and (b) k=10 amu/ps<sup>2</sup>

In the case of k=1, the wall is not solid enough to prevent the fluid atoms from penetrating it while the k=10 wall maintains its solidity sufficiently. From this type of evaluation and using the Lindemann criterion, it was determined that the lattice spring constant must be at least 10 amu/ps<sup>2</sup>.

Then the effect of the spring constant on the energy transfer rate was considered. It is desirable for frictional heat to be transferred efficiently out of the fluid in a molecular simulation because this models the macroscopically observed conduction of heat out through metal surfaces. This can be measured as a function of the steady state temperature of the fluid. Lower steady state fluid temperature corresponds to more heat being transferred out of the fluid. This trend of increasing fluid temperature with increasing spring constant is illustrated in Figure 6-4.



Figure 6-4: Steady state fluid temperature as a function of the wall lattice spring constant.

As has been observed before (Cui et al. 1999), larger values of k correspond to slower energy transfer from the fluid to the walls. Based on this analysis, the value of the lattice spring constant was chosen to be k=10 amu/ps<sup>2</sup>.

#### 6.3.4 The Fluid Model

The lubricant modeled in most simulations utilized in this research is n-decane. This choice was made based on the fact that n-decane is an often modeled fluid in molecular simulation and many references are available for results comparison. One reason that n-decane molecule is a popular choice is that the viscosity-shear rate power law coefficient has been consistently found to be -2/3 using both constant pressure and constant volume simulations (Balasundaram et al. 1999).

The n-decane molecule consists of a chain of eight methylene (CH<sub>2</sub>) and two methyl

(CH<sub>3</sub>) groups. However, not all of the atoms in the molecule are modeled explicitly in order to save computational time. The hydrogen and carbon atoms are combined into a single united atom having composite properties. The interaction parameters of the united atom are defined to incorporate the effects of the component atoms (Leach 2001). Use of the united atom model is common practice in thin film molecular simulations (Khare et al. 1996; Jabbarzadeh et al. 1998; Zhang et al. 2001).

The fluid molecules are subject to bond bending and twisting (torsion). The potential used to model the deviation of bond angles from their reference value is the cosine harmonic potential given in Equation 6.4 (Balasundaram et al. 1999).

$$\Phi_{bending} = \frac{1}{2} k_{\theta} \left( \cos \theta_i - \cos \theta_{equlibrium} \right)$$
(6.4)

In the bond bending potential,  $k_{\theta}$  is an angle spring constant, and  $\theta_{equilibrium}$  is the equilibrium bond angle. For the Carbon-Carbon bonds that make up the backbone of n-decane, the values for these constants are  $k_{\theta} = 124$  kcal/mol and  $\theta_{equilibrium} = 114$  K (Macedonia and Maginn 1999). The potential used to model torsion is a cosine expansion as given in Equation 6.5 (Balasundaram et al. 1999).

$$\Phi_{torsion} = \sum_{n=0}^{3} V_n (\cos \phi)^n \tag{6.5}$$

In the torsion model of four bonded Carbon atoms, the constants in Equation 2.14 are  $V_0 = 2.00642$ ,  $V_1 = 4.01084$ ,  $V_2 = 0.27092$ , and  $V_3 = -6.28819$  kcal/mol (Macedonia and Maginn 1999).

#### 6.3.5 Initial Fluid Density

A grand canonical Monte Carlo (GCMC) simulation was used to calculate the initial density of the fluid molecules prior to the start of the MD simulation. In the grand canonical ensemble the chemical potential, the volume, and the temperature are constant (Leach 2001). The number of particles fluctuates, and the simulation involves inserting, deleting, and translating molecules. The primary input parameters in the GCMC simulation are fugacity (or chemical potential), temperature, and volume of the space between the confining walls.

Fugacity is a measure of the effective pressure for real fluids (Atkins 1978). To run a simulation at a predefined pressure, the pressure must first be converted to fugacity. First the liquid compressibility, *Z*, is calculated using the cubic form of the Peng-Robinson equation 2.of state given in Equation 6.6 (Sandler 1999).

$$Z^{3} - (1 - B)Z^{2} + (A - 3B^{2} - 2B)Z - (AB - B^{2} - B^{3}) = 0$$
  

$$B = bp/RT \quad A = ap/R^{2}T^{2}$$
(6.6)

In this expression, a and b are functions of the critical temperature, critical pressure, acentric factor, and boiling point of the fluid, and R is the gas constant. From the compressibility, the fugacity, f, can be calculated using the expression for liquid fugacity given in Equation 6.7 (Sandler 1999).

$$\ln\frac{f}{P} = (Z-1) - \ln\left(Z - \frac{bP}{RT}\right) - \frac{a}{2\sqrt{2}bRT} \ln\left[\frac{Z + (1+\sqrt{2})bP/RT}{Z + (1-\sqrt{2})bP/RT}\right]$$
(6.7)

Atmospheric pressure (1 atm) and room temperature (300K) are input into Equation 6.7 as P and T respectively, and the fugacity can be calculated.

After these calculations are complete, a GCMC simulation can be run until it converges at which time the fluid molecules will be in an equilibrium state for the input fugacity, film thickness, and temperature. Convergence is measured by evaluating the average number of molecules in the simulation cell. An example of this convergence is illustrated in Figure 6-5, which plots the average number of fluid molecules as a function of GCMC steps.



Figure 6-5: Example of the equilibration of the average number of fluid molecules in a typical GCMC simulation.

In this case, the average number of molecules converges to 19 after approximately 2 million steps. The simulation is considered to be converged when the fluctuations in the number of average fluid molecules is less than the square root of the average number of molecules divided by the average number of molecules (Haile 1992). For this example, the convergence criteria is

 $\sqrt{\langle N_{molecules} \rangle}/\langle N_{molecules} \rangle = \sqrt{19}/19 \approx 0.23$ . The initial configuration of fluid atoms for the MD simulation can be taken from any GCMC configuration after this convergence is obtained where the instantaneous number of molecules is at its equilibrium value.

#### 6.3.6 Interaction Potentials

The interactions between two wall atoms, a wall atom and a fluid atom, two fluid atoms in different molecules, and two fluid atoms in the same molecule separated by at least three bonds are modeled by the Lennard-Jones potential energy function. This function is given in Equation 6.8.

$$\Phi_{LJ}(r) = 4\varepsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^{6} \right]$$
(6.8)

This potential model simulates van der Waals interactions as close range repulsive forces and long range attractive forces. The interaction is dependant on the values of the two adjustable parameters,  $\sigma$  and  $\varepsilon$ . The Lennard-Jones distance parameter,  $\sigma$ , is the distance at which there is zero potential energy. The Lennard-Jones energy parameter,  $\varepsilon$ , is the minimum energy (Haile 1992). This model was chosen because it is the most commonly used in MD simulations of this type. The values of the Lennard Jones parameters for the fluid-fluid interactions are based on tabulated parameters for the united atom models of methyl and methylene. These values are  $\sigma_{CH2-CH2} = 3.93$  A and  $\varepsilon_{CH2-CH2} / k_B = 47K$  for mythylene, and  $\sigma_{CH3-CH3} = 3.77$  A and  $\varepsilon_{CH3-CH3} / k_B = 98.1K$  for methyl (Macedonia and Maginn 1999).

The values of the Lennard-Jones parameters for the simulated wall-fluid interactions are not currently representative of a physical interaction. Typically, researchers have used multiples of the fluid-fluid interaction parameters. Parameters that are frequently used are  $\sigma_{wf}=\sigma_{ff}$  and  $\varepsilon_{wf}=4\varepsilon_{ff}$  (this has been suggested as an approximation of interactions of mica surfaces) (Jabbarzadeh et al. 1998). These parameters will be used initially in this research in order to replicate existing research as closely as possible for model verification. However, as the research progresses, it is anticipated that the Lennard-Jones potential will be replaced by a better model of solid atom interactions.

The parameters for interactions between methyl and methylene are calculated using the Lorentz-Berthelot mixing rules given in Equation 6.9.

$$\sigma_{CH2-CH3} = \frac{1}{2} (\sigma_{CH3} + \sigma_{CH2})$$

$$\varepsilon_{CH2-CH3} = \sqrt{\varepsilon_{CH3} \varepsilon_{CH2}}$$
(6.9)

#### 6.3.7 Heat Generation/Dissipation

The frictional heat added to the system by the wall shear is removed by the wall thermostat. Therefore, in an accurate, converged simulation, the viscous heat generated should be comparable to the heat dissipated by the thermostat per unit time (Gupta et al. 1997; Balasundaram et al. 1999). This analysis can be performed by comparing the energy added to the system due to viscous heating to the energy expended by the thermostat to remove that heat.

The energy associated with the Nose-Hoover thermostat used in this simulation is the sum of the kinetic and potential energies of the extended coordinate, s (Allen and Tildesley 1987). These energies are calculated using the expressions given in Equation 6.10.

$$\Phi_{s} = (f+1)k_{B}T\ln s$$

$$K_{s} = \frac{1}{2}Q\dot{s}^{2} = p_{s}^{2}/2Q$$
(6.10)

The rate at which the thermostat expends energy is then just the total extended kinetic and potential energy  $(\Phi_s + K_s)$  divided by the duration of the simulation. The rate of heat generation due to the wall shear can be calculated from the intensity of viscous heating multiplied by the fluid volume. The viscous heating intensity is related to the shear stress and strain rate as given in Equation 6.11 (Stachowiak and Batchelor 2001).

$$S = \eta \left(\frac{du}{dz}\right) = \frac{\tau_{xz}}{du/dz} \left(\frac{du}{dz}\right) = \tau_{xz} \left(\frac{du}{dz}\right) = \tau_{xz} \cdot \dot{\gamma}$$
(6.11)

The shear stress,  $\tau_{xz}$ , is calculated using the virial expression (Wang and Fichthorn 2002) and the strain rate,  $\dot{\gamma}$ , is obtained from the average fluid velocity profile. The result of the comparison between thermostat energy rate and the rate of viscous heating is illustrated in Figure 6-6.



Figure 6-6: Rate of energy added/removed due to viscous heating (blue triangles) / thermostat (pink squares) as a function of applied shear rate

The rate of energy added to the system due to the viscous heating is comparable to the rate of energy expended by the thermostat to remove that heat. This consistency is indicative of a successful simulation.

#### 6.4 Conclusions

The MD simulation tool described in this section was validated prior to use for new research by comparison of observed behaviors with trends reported in the literature. This validation included analyses of the effect of simulation parameters such as wall-fluid interaction strength, wall temperature, and wall speed on measured properties such as density, viscosity, interface slip, and steady state fluid temperature. The validated simulation can now be employed to investigate the behavior of the thin film density, solvation pressure, interface slip, and thin film viscosity. It can be assumed that the simulation details given in this chapter are applicable to all subsequent chapters unless otherwise specified.

# Chapter 7 Thin Film Density

### 7.1 Background

The first thin film property characterized using the simulation detailed in the previous chapter to be discussed is fluid density. The density of a fluid confined to a nano-scale gap may exhibit behavior different than that of the same fluid in the bulk. There are two primary differences that have been reported in the literature. These are the formation of the fluid into discrete layers parallel to the solid walls and a decrease of average density with decreasing channel width. These phenomena have been investigated using molecular simulation tools for many years. Researchers have employed both Monte Carlo (Snook and van Megen 1979; Somers and Davis 1992; Ayappa and Chandana 2002; Pertsin and Grunze 2003) as well as molecular dynamics (Khare et al. 1996; Gupta et al. 1997; Jabbarzadeh et al. 1998; Wang and Fichthorn 2002). Confined fluid density behavior has also be predicted using theoretical approaches - specifically density functional theory (Tarazona and Vicente 1985; Attard and Parker 1992; Mitlin and Sharma 1995). More recently, advances in instrumental and experimental techniques have enabled thin film density to be investigated using direct experimentation. Experimental approaches have included use of an extended surface force apparatus (Heuberger et al. 2001) and various techniques using x-ray technology (Huisman et al. 1997; Yu et al. 1997).

This chapter will introduce the basic behavioral characteristics of density in confined films. The phenomena of molecular layering parallel to the channel walls and density decrease

with decreasing channel width will each be briefly described and illustrated using data from the author's simulations. Although detailed analyses will not be performed, it is necessary to nominally present observed trends since most of the unique behaviors of thin films that will be discussed in subsequent chapters can be directly correlated to the density phenomena described here.

#### 7.2 Discrete Fluid Layers

A common method for analyzing the structure of confined fluid is using density profiles. Density profiles can be calculated from the average position of the atoms over the duration of a molecular simulation (in this research, either the GCMC or MD simulation can be used). The volume between the confining walls is divided into many thin layers of constant width, hereafter referred to as "bins". Then, for each simulation step, the number of atoms (united atoms here) in each bin is counted. This number, average over the entire simulation yields the density profile. An example of a snapshot of an MD simulation at a single step and the corresponding average density profile are illustrated in Figure 7-1.



Figure 7-1: Example of a snapshot of a simulation at a single time step (left) and the average density profile obtained using bins 0.05 nm wide (right) in a 2 nm channel.

In this example, the fluid forms, on average, four discrete fluid layers parallel to the confining walls. Discrete layering is observed in fluids confined to channels on the same order of magnitude as the fluid molecule/atom. The number of layers increases as the channel width increases. This is illustrated from the plot of the number of fluid layers as a function of channel width from the author's simulations in Figure 7-2.



Figure 7-2: Average number of fluid layers increasing with channel width and corresponding representative density profiles with 1, 2, 3, and 4 fluid layers.

At large channel widths, molecules far from the walls exhibit essentially bulk behavior and do not form discrete layers (Pertsin and Grunze 2003). Layering plays a critically important role in thin film behavior and directly affects many different properties of the confined fluid. As will be discussed in detail throughout the following several chapters, layering is integrally related to solvation pressure, interface slip, and effective viscosity.

#### 7.3 Mean Density Decrease

The density of a confined fluid can also be evaluated as an average value across the channel (as opposed to a density profile). It has been observed both experimentally (Heuberger et al. 2001) and via molecular simulation (Snook and van Megen 1980; Pertsin and Grunze 2003)

that the average density of a confined fluid is less than that of the same fluid in the bulk. The decrease of density with decreasing channel width has been attributed to the effect of excluded volume (Heuberger et al. 2001; Pertsin and Grunze 2003). In the general sense, excluded volume is the volume surrounding a given object that is excluded to another object. In the case of confined fluids, it specifically refers to the space immediately next to a confining wall that is excluded to the fluid molecules.

Using excluded volume theory, the confined fluid average density,  $\overline{\rho}$ , can be approximated as the bulk density  $\rho_{Bulk}$  multiplied by the ratio of the excluded volume to the total volume. At constant area, this volume ratio can be replaced by a distance ratio and the average density is calculated

$$\overline{\rho} = \rho_{Bulk} \cdot \left[\frac{h - h_e}{h}\right] \tag{7.1}$$

It has been suggested that the value of the excluded distance,  $h_e$ , should correlate with the width of the excluded region in the fluid density profile (Pertsin and Grunze 2003). To evaluate this possibility, we have obtained average density data from the literature. The following is a plot of the average density in a confined fluid normalized by the bulk density at a range of channel widths from various references.



Figure 7-3: Average density in a confined fluid normalized by the bulk density of that fluid as a function of the channel width normalized by the characteristic size of the fluid molecule. Data from GCMC simulation of Lennard-Jones fluid and walls - filled triangles (Pertsin and Grunze 2003), filled squares (Somers and Davis 1992), and empty triangles (Snook and van Megen 1980). Data from GCMC simulation of methane in graphite walls – empty circles (Ayappa and Chandana 2002). triangles Data from MD simulation of ndecane molecules between Lennard-Jones walls - filled circles (Wang and Fichthorn 2002). Experimental data of cyclohexane between mica sheets using a surface force apparatus blue diamonds (Heuberger et al. 2001).

Fitting Equation 7.1 to the data in Figure 7-3 enables estimation of the excluded volume. The value obtained using a least squares fit is  $h_e = 0.3 \sigma$ . This indicates that there is a distance approximately 0.15  $\sigma$  away from each wall that is unoccupied by the first fluid layer. In small channels this distance is comparable to the total channel width and therefore the average density

of the fluid is reduced. However, in large channels, the excluded distance is small compared to the total width of the channel and the average fluid density approaches the bulk value.

### 7.4 Conclusions

The density of a confined fluid may be quite different from the same fluid in the bulk due to the formation of discrete layers and excluded volume effects resulting in a decrease of the average density. These two behaviors were presented briefly in this chapter using molecular dynamics simulation data. The effects of these behaviors, particularly those of fluid layering, on the unique characteristics and properties of confined fluids will be referred to frequently in subsequent chapters.

# Chapter 8 Solvation Pressure

#### 8.1 Background

Another behavior unique to fluids confined to nano-scale channels is solvation pressure. This is an additional component of pressure that acts perpendicular to the confining walls and oscillates with variable channel width. Solvation pressure can be related to the layered density profiles discussed in the previous chapter and is thought to arise when the ordering of fluid molecules into discrete layers is disrupted due to the confinement (Isrealachvili 1992). Although the relationship between discrete fluid behavior and solvation pressure is understood conceptually, models that can predict solvation pressure quantitatively are necessary to incorporate solvation pressure into interface design. Significant efforts have been made towards this goal using experiment, molecular simulation, and theoretical approaches. Experimental methods can be used to determine the solvation force by measuring the deflection of a spring that supports a fluid-confining channel wall (Horn and Isrealachvili 1981). Predictive models are then developed by fitting experimental data to empirical expressions. Typically the form of these expressions is an exponentially decaying cosine function with at least two empirical constants (Chan and Horn 1985; Abd-AlSamieh and Rahnejat 2001). Solvation pressure has also been characterized by atomistic Monte Carlo (Snook and van Megen 1980; Porcheron et al. 2002; Pertsin and Grunze 2003) and molecular dynamics (Wang and Fichthorn 2002; Martini et al. 2006) simulations. In simulation studies, solvation pressure is calculated from the positions

and velocities of particles averaged over typically lengthy simulations. The disadvantages of using molecular simulation or experiment-based approaches for application design are the relatively slow speed with which results can be obtained and that the resultant models are often applicable only to a specific system or set of operating conditions.

Theoretical approaches have also been employed. These approaches typically calculate solvation pressure from fluid density profiles predicted using density functional theory (Tarazona and Vicente 1985; Attard and Parker 1992; Mitlin and Sharma 1995). The advantage of theoretical models is their relative efficiency and flexibility. This work proposes an enhancement to such models based on the observation that the dominant component of the solvation force is due to interactions between a wall and the fluid layer immediately next to it. The relationship between solvation pressure and the distance between the channel wall and first liquid layer is investigated using molecular simulation. Then the Hamaker summation method is used to quantify this relationship. This formulation enables prediction of solvation pressure using a single data point – the distance between the wall the first fluid layer (as opposed to a complete density profile). The relationship between solvation pressure and the wall-fluid layer distance is validated using two different molecular simulations.

#### 8.2 Observations

Solvation pressure is calculated from molecular dynamics simulations run with channels widths between 0.6 and 3 nm using the virial expression (Wang and Fichthorn 2002). The resultant solvation pressure is observed to oscillate with channel width where the periodicity is comparable to the fluid atomic size and the amplitude decays with increasing channel width. This behavior is consistent with that reported by other researchers using both experiment

(Christenson 1983; Chan and Horn 1985) and molecular simulation (Snook and van Megen 1980; Wang and Fichthorn 2002). It has also been observed both in this research and others (Tarazona and Vicente 1985) that, for the small channel widths at which solvation pressure is significant, the dominant component of the solvation force is due to interactions between a wall and the fluid layer immediately next to it. This interaction force is a function of the separation distance between the wall and fluid layer.

The distance between the wall and the first fluid layer, r, can be measured directly from the atomic density distributions (calculated as an average over the duration of the simulation after steady state is obtained) as a function of the channel width, h. At large channel widths, this layer distance reaches a constant, equilibrium value,  $r(h \rightarrow \infty) = r_0$ . However, for fluids confined to a small number of layers, the wall-fluid layer distance varies with channel width. The difference between the wall-fluid layer distance at a given channel width and the equilibrium distance will be defined as  $\Delta r = r - r_0$ . The sign of  $\Delta r$  indicates whether the wall-fluid layer distance. For several representative channel widths, a snapshot of the simulation cell at a single moment in time, the average density profile, and the percent difference of the wall-fluid layer distance from equilibrium are given in Table 8-1.

Table 8-1: Illustration of the molecular layering and wall-fluid layer distance for ndecane fluid confined in channels of widths of 0.9, 1.1, 1.3, 2.0, and 3.0 nm. For this system the equilibrium wall-fluid layer distance is  $r_0 = 0.234$  nm.

<i>h</i> (nm)	Simulation Snapshot	Average Density Profile	$\Delta r/r_0$
0.9			-1.87%
1.1			2.43%
1.3			-1.35%
1.5	nesesterne henselfter estrentet Enterneteningen gint för som det ander handen statesternet inderede		0.84%
2	Serie - Star - Star Star - Star - St		0.02%
3			-0.04%

The percent difference from equilibrium in the far right column of Table 8-1 oscillates with channel width between negative, where the wall-layer distance is smaller than the equilibrium value (e.g. h=0.9 nm), and positive, where the wall-layer distance is larger than the equilibrium value (e.g. h=1.1 nm). In addition, the magnitude of the difference from equilibrium decreases with increasing channel width. This behavior is a result of the fact that, at large channel widths, molecules far from the walls do not form discrete layers and exhibit essentially bulk behavior (Pertsin and Grunze 2003), as can be observed in the simulation snapshot of the 3nm channel.

This periodic wall-fluid layer distance is observed to correlate with the oscillatory behavior of solvation pressure as shown in Figure 8-1. This figure illustrates that the wall-layer distance and the solvation pressure oscillate as a function of channel width with the same wavelength, but that they are inversely related. That is, large positive solvation pressures correspond to wall-fluid layer distances that are smaller than the equilibrium value. A similar relationship can be inferred from Figure 2 of (Porcheron et al. 2002) in which density profiles for methane films are depicted for the channels widths at which the maximum and minimum solvation pressure occur.



Figure 8-1: Average difference between the wall-fluid layer distance and the equilibrium distance (top) and the solvation pressure (bottom) as functions of channel width. Periodicity that is common to both wall-fluid layer distance and solvation pressure is highlighted by shaded bars. Channel widths corresponding to 2, 3, and 4 fluid layers are also indicated in the upper plot.

Next, the physical origin of the variations of wall-fluid layer distance and solvation pressure with channel width will be investigated. It has been observed that confined fluids tend to form an integer number of discrete layers (Snook and van Megen 1980; Horn and Isrealachvili 1981; Christenson 1983; Isrealachvili 1992; Matsuoka and Kato 1997). Therefore, a fluid confined between two solid surfaces will be comprised predominantly of layers. Figure 8-2 illustrates conceptually, for a case of two fluid layers, how confinement and discrete layering

lead to a variable wall-fluid layer distance. If the distance between the walls is too small (Figure 8-2, Left), the fluid molecules exert a force on the walls that tends to push them apart. This condition, corresponding to a positive solvation pressure by convention, will be referred to as "deficit space". If the distance between the walls is too large, but not yet large enough for an additional fluid layer to form (Figure 8-2, Right), the fluid molecules exert a force that tends to pull the walls together. This case will result in a negative solvation pressure and will be referred to as "excess space". In between deficit and excess space, there is a channel width at which the system is in mechanical equilibrium (Figure 8-2, Center), and the corresponding solvation pressure is zero.



Figure 8-2: Conceptual illustration of the relationship between channel width, number of discrete fluid layers, and wall-fluid layer distance. Deficit Space,  $r < r_0$ : Two discrete fluid layers confined to a small channel width resulting in a positive (repulsive) solvation

pressure. Equilibrium Spacing,  $r = r_0$ : Two discrete fluid layers confined to an equilibrium channel width resulting in zero solvation pressure. Excess Space,  $r > r_0$ : Two discrete fluid layers confined to a large channel width (yet not big enough for three fluid layers) resulting in negative (attractive) solvation pressure.

#### 8.3 Analysis

The wall-fluid layer distance can be related quantitatively to solvation pressure using pairwise additivity, also referred to as the Hamaker summation method (Isrealachvili 1992), where the interaction energy per unit area between two multi-atom bodies, W, is calculated as the sum of the individual atom-atom interaction energies. The form of the resultant "two-body" potential is a function of the geometry of the two bodies. In a confined film, the wall and first fluid layer serve as the two bodies, which can be represented as two interacting planar surfaces. For this geometry, the total energy per unit area when the surfaces are a distance r apart is

$$W = -\frac{2\pi C\rho_w \rho_f}{(n-2)(n-3)(n-4)r^{n-4}}$$
 where  $\rho_w$  and  $\rho_f$  are the number density of the wall and fluid

layer respectively and *C* and *n* are parameters defined by the atom-atom pair potential (Isrealachvili 1992). For the attractive component of the Lennard-Jones atom-atom pair potential,  $C = 4\varepsilon\sigma^6$  and n = 6, and for the repulsive component,  $C = -4\varepsilon\sigma^{12}$  and n = 12. Therefore, the total interaction energy per unit area for two planar surfaces using the Lennard-Jones potential energy function is

$$W = \pi \varepsilon \rho_w \rho_f \left[ \frac{\sigma^{12}}{90r^8} - \frac{\sigma^6}{3r^2} \right]$$
(8.1)

The pressure (i.e. force per unit area) can be calculated by taking the derivative of the energy per unit area,  $P_s = -\partial W(r)/\partial r$ . In this case, the solvation pressure corresponding to Equation 8.1 is

$$P_{S} = \pi \varepsilon \rho_{w} \rho_{f} \left[ \frac{4\sigma^{12}}{45r^{9}} - \frac{2\sigma^{6}}{3r^{3}} \right]$$

$$(8.2)$$

The equilibrium layer distance at which the solvation pressure is zero can be calculated from this expression,  $r_0 = (2/15)^{\frac{1}{6}} \sigma$ .

When the first layer is at its equilibrium distance (i.e.  $r = r_0$ ) the solvation pressure calculated using Equation 8.2 is zero as expected. When the fluid layer is closer to the wall (i.e.  $r < r_0$ ) the solvation pressure is positive, and when the layer is further from the wall (i.e.  $r > r_0$ ) the opposite is true. In the limiting case of infinite wall-fluid layer distance, the solvation pressure will go to zero. The other limit occurs when the wall-fluid layer distance goes to zero, which would result in an infinitely large positive (repulsive) solvation pressure. These analyses indicate that the expected limiting-case behavior of the solvation pressure is accurately captured by Equation 8.2.

The next step is to evaluate the validity of the developed relationship between solvation pressure,  $P_S$ , and the wall-fluid layer distance, r. This can be done by measuring r from the simulation density profiles, calculating  $P_S$  from Equation 8.2, and then comparing the calculated value to that obtained from the simulation. The density of the face-centered cubic lattice wall can be calculated using geometric arguments as  $\rho_w = 5.84 \times 10^{28} m^{-3}$ . The fluid density calculation is slightly more complicated because the density is not homogeneous throughout the

channel. In confined fluids, the fluid layer near the wall has been observed experimentally to be denser than the fluid in the bulk (Horn and Isrealachvili 1981). The difference between the first layer density and the bulk density can be seen from the representative atomic density distribution for n-decane shown in Figure 8-3. This figure illustrates a density profile (averaged over the simulation time) for a 5 nm channel width that contains both the high density fluid layer next to the wall and a bulk fluid region in the middle. In this case, the first fluid layer density is approximately five times that of the bulk. Since it is this first layer that is assumed to dominate the solvation pressure in the present model, the fluid density used to calculate the solvation pressure is that of the first fluid layer (i.e. five times the bulk density,  $\rho_f = 1.53 \times 10^{29} m^{-3}$ ).



Figure 8-3: Fluid (united) atomic density distribution for n-decane averaged over a simulation run with a channel width of 5 nm. The density of the first fluid layer is approximately 5 times that of the bulk fluid region in the middle of the channel. The volume of each bin is the 2.57 nm<sup>3</sup>.

The wall-fluid layer distances measured from the simulation and the approximate densities of the wall and fluid layer are used in Equation 8.2 to calculate the solvation pressure. A comparison of the solvation pressure obtained from the molecular simulations and that calculated from the wall-fluid layer distances is illustrated in Figure 8-4. Although there is some difference between the simulation results and those estimated by the present model, the trends are captured well and the order of magnitude of the estimation is correct. This indicates that the proposed relationship between wall-fluid layer distance and solvation pressure exists in these simulations. It is

important to note that although these results are for n-decane with 10 monomers, results can be expected to be the same for un-branched polymer chains of different lengths based on observations from both molecular simulation and density functional theory that changing the number of monomers does not greatly affect density profiles (Khare et al. 1996).



Figure 8-4: Solvation pressure for n-decane as a function of channel width obtained by averaging simulation results at different wall speeds (triangles) and calculated from the wall-fluid layer distance (solid line).

To ensure that these findings are not specific to our simulation, the relationship between wall-fluid layer distance and solvation pressure was evaluated for an additional case. (Snook and
van Megen 1980) reported both density profiles and solvation pressure obtained from grand canonical Monte Carlo simulations of simple spherical atoms confined between planar walls. In that research, the wall and fluid atoms have the same Lennard-Jones parameters, which are similar to those of argon. All simulation parameters are normalized by the interaction potential constants,  $\sigma$  and  $\varepsilon$ . The average wall-fluid layer distance can be estimated from the density profiles in Figures 2 and 3 of that work (Snook and van Megen 1980). The fluid walls are constructed of argon atoms in a face-centered cubic lattice and therefore have a reduced density of  $\rho_{w*} = 1.4\sigma^{-3}$ . Density profiles reported by (Snook and van Megen 1980) (see Figure 2 of their paper) confirm that the density of the first fluid layer is approximately five times the bulk density,  $\rho_{f*} = 5(0.59\sigma^{-3}) = 2.96\sigma^{-3}$ . The solvation pressure is calculated at each channel width for which density profiles are given using a normalized form of Equation 8.2. In Figure 8-5, the results of this calculations are compared to the data reported by (Snook and van Megen 1980) (see Table 1 of their paper). Some inconsistency can be observed. However, it may be, in part, attributed to the resolution of the density profile images and the therefore error in extracting the wall-fluid layer distances. In addition, the calculated curve contains only seven data points

(extracted from the seven reported density profiles from (Snook and van Megen 1980)) which limits its ability to fully capture periodic behavior. However, the period, amplitude, and decay

rate of the solvation pressure are captured quite well.



Figure 8-5: Solvation pressure versus channel width: comparison of results reported by (Snook and van Megen 1980) from simulation (hollow squares) and predicted from the wall-fluid layer distance (solid line). Results are presented in dimensionless form as indicated.

### 8.4 Conclusions

Analyses using molecular simulation revealed a relationship between the behavior of solvation pressure and variations in the distance between a channel wall and the first fluid layer. This relationship was quantified using the Hamaker summation method which enabled comparison of simulation measured solvation pressure to that calculated from the wall-fluid layer distance. Agreement between the two confirmed the validity of both the relationship and the quantification method. These results provide a means of calculating solvation pressure from a

single parameter, the distance between the wall and the first fluid layer, and thereby simplifying predictive capabilities using theoretical models.

# Chapter 9 Interface Slip

# 9.1 Background

Interface slip, a difference between a wall and the fluid immediately next to it, is another important area of thin film research. A classical observation in fluid dynamics is the no-slip condition, which finds that the fluid adjacent to a stationary solid boundary is also, on average, stationary. Though this condition remains trustworthy for large-scale flows of Newtonian fluids, recent reviews of physical experiments as well as computer simulations (for examples see references in (Neto et al. 2005) and (Zhu and Granick 2001)) document that the no-slip condition is not universal. Fluids can slip relative to solids, and slip is especially prominent in small-scale flows. Therefore, understanding and quantifying slip between the solid and lubricant in thin film lubrication is extremely important for prediction of interface behavior.

Many different experimental, simulation, and theoretical approaches have been employed in order to understand and characterize the slip phenomenon. Experimental approaches typically employ either a surface force apparatus or an atomic force microscope. In both cases, slip can be inferred from force drainage measurements. Alternative approaches are fluorescence recovery which is an optical technique for obtaining near wall velocity measurement, or acoustic wave devices where slip is calculated from changes in the acoustic load impedance. Some experimental slip investigations prominent in the literature are (Cottin-Bizonne et al. 2002; Sun et al. 2002; Choi et al. 2003; Leger 2003; Neto et al. 2005; Huang et al. 2006). Molecular simulation has also been identified as a powerful tool for investigating slip behavior. These typical involve non-equilibrium molecular dynamics simulation in which slip can be measured directly by calculating average particle velocities. Some examples from the literature include (Koplik et al. 1989; Khare et al. 1996; Manias et al. 1996; Gupta et al. 1997; Jabbarzadeh et al. 1999; Cieplak et al. 2001; Priezjev and Troian 2004). Come recent simulation-based slip investigations have also employed the lattice-Boltzmann model (Benzi et al. 2006; Szalmá 2006). All of these studies reveal that the velocity of the first liquid layer in a nano-confined fluid cannot be assumed to have the same velocity as the solid next to it.

In this research, molecular dynamics simulation is used to explore slip behavior. Slip can be measured from molecular dynamics simulation from the average velocity profile. The volume between the walls is divided into "bins" as described in the Density chapter of this dissertation. Then the velocity profile is generated from the average velocity of the atoms in each bin. Figure 9-1 illustrates the relationship between a snap shot of the simulation at a single moment in time, an average density profile, and an average velocity profile. Note that the velocity profile is only taken from regions where the atomic density is large enough that averaging makes sense. Figure 9-1 also identifies the fluid shear rate taken from the linear velocity profile of the interior layers and the speed of the first fluid layer.



Figure 9-1: Snapshot of the simulation at a single time step (left), and the density (center) and velocity (right) profiles averaged over the duration of the simulation after Monte Carlo equilibration. The average shear rate,  $\langle \dot{\gamma} \rangle$ , and velocity of the first fluid layer,  $\langle v_{liquid} \rangle$ , are indicated on the velocity profile.

The degree of slip can be quantified by slip length,  $L_S$ . For Couette flow, this is defined by first extrapolating the fluid velocity profile to the wall. In a frame of reference that is stationary, velocity extrapolated to the wall is called the slip speed,  $v_S$ . If the slip speed is nonzero, that the extrapolation can be extended until its value reaches zero. The depth below the wall at which the slip velocity is equal to zero is called the slip length.

The existence of slip in the molecular simulation can be illustrated by comparing the applied shear rate (i.e. the relative wall speed divided by the channel width) to the average shear rate of the fluid. This comparison is shown in Figure 9-2.



Figure 9-2: Shear rate as a function of channel width. Solid shapes correspond to applied shear rate data points while hollow shapes represent the average fluid shear rate.

It can be observed that at this range of channel widths the fluid shear rate is less than the applied shear rate. It can also be observed that the difference between the applied and fluid shear rates increases as the channel width decreases in size indicating that slip is more significant in smaller channels. The difference between applied and average fluid shear rate is directly related to the magnitude of the interface slip.

In this chapter, molecular simulation is utilized to further investigate the behavior and origin of solid-fluid interface slip. These investigations include comparison of relationship between slip magnitude and shear rate reported in the literature and analysis of potential reasons for observed discrepancies in the results; evaluation of the effect of scaling slip length by system size; identification of the location of slip and explanation of this behavior in terms of the relative magnitude of the solid-fluid friction as compared to the fluid-fluid friction; and analysis of the relationship between slip magnitude and solvation pressure and interpretation of this relationship by viewing slip as a rate process. Some of the content of the last section discussing the relationship between solvation pressure and slip is also available in (Lichter et al. Accepted).

### 9.2 Comparison of Reported Results

Slip behavior is often evaluated in terms of the affect of shear rate on slip magnitude. Here, several studies have been chosen from the literature that report this magnitude, namely Jabbarzadeh et.al. (Jabbarzadeh et al. 1999), Khare et.al. (Khare et al. 1996), Priezjev and Troian (Priezjev and Troian 2004), and Gupta et.al. (Gupta et al. 1997). In addition, slip data was obtained from the simulations described in this dissertation. These literature references were chosen because of the similarities of their simulations. In all cases, non-equilibrium molecular dynamics was used to simulate Couette flow.

In most simulations, the upper and lower walls were moved in opposite directions, while in one study only one wall was moved. These two different appearing geometries are equivalent through a Galilean transformation in the flow direction. The fluids were polymers consisting of between two and thirty united atoms. Atomic interactions were modeled using the Lennard-Jones potential model. A summary of the critical simulation parameters for each reference is given in Table 9-1. Table 9-1: Summary of non-equilibrium molecular dynamics simulations for the compared references. If no value is listed, "n/a" indicates that the parameter is not applicable to a particular simulation or "-" indicates that the parameter is not specified in the reference.

	(Jabbarzadeh	(Khare	(Priezjev	(Gupta	(Martini
	et al. 1999)	et al.	and Troian	et al.	et al.
		1996)	2004)	1997)	2006)
Potential Parameters					
Fluid Well Depth, $\sigma$ (nm)	0.405	0.393	-	0.393	0.393
Fluid Min Energy, ε/k <sub>b</sub> (K)	50.5	47.0	-	47.0	47.0
Wall-fluid $\sigma_{wf}$ ( $\sigma$ )	1.00	-	0.75	0.56	0.84
Wall-fluid $\varepsilon_{wf}$ ( $\varepsilon/k_b$ )	1.00	-	0.60	1.70	0.34
Confining Walls					
Number moving walls	2	2	1	2	2
Wall lattice	bcc	Fcc	fcc	n/a	Fcc
Wall flexibility	Yes	Yes	No	n/a	Yes
Polymer Properties					
Chain Length, N	16	20	2-16	24, 30	10
Fluid density ( $\sigma^3$ )	2.29	0.80	0.81	0.82	1.73
Atomic Mass, m (amu)	14.12	-	-	14.00	14.00
<b>Operating Conditions</b>					
	9.64	18.00	24.57	9.25	2.54-
Wall separation, $h(\sigma)$					6.87
Wall temperature ( $\varepsilon/k_b$ )	9.46	4.00	n/a	n/a	6.38
	9.46	4.80	1.10	6.38	6.38-
Fluid temperature ( $\varepsilon/k_b$ )					30.91
Min Wall Speed $(\sqrt{\varepsilon/m})$	0.06	0.07	0.05	0.05	0.06
Max Wall Speed $(\sqrt{\varepsilon/m})$	35.75	6.95	2.53	0.50	5.99

The dependence of slip length on shear rate is typically reported in terms of variables normalized by the length and time scale of the simulation. The slip length is normalized by the characteristic size of the fluid atoms,  $L_S = L_S / \sigma$ . And the shear rate is normalized by the

characteristic atomic collision time,  $\dot{\gamma} = \dot{\gamma}\tau = \dot{\gamma}\sqrt{m\sigma^2/\varepsilon}$ , where *m* is the characteristic mass of a monomer and  $\varepsilon$  is the Lennard-Jones energy of the atom-atom interactions.



Figure 9-3: Slip length as a function of shear rate (normalized by the atomic length and time scales). Lines have been added to distinguish the different sets of data from: 1. (Khare et al. 1996), 2. (Priezjev and Troian 2004), 3. (Jabbarzadeh et al. 1999), 4. (Gupta et al. 1997), and 5. author's simulations.

Note that not all of the references directly reported slip length. In some cases, a different measure of slip was reported, and the slip length had to be calculated from the parameter in order to produce Figure 9-3.

This comparison reveals variation in both the magnitude of slip length and its relationship to shear rate. In addition, the authors of these references interpret and explain their results using very different arguments. (Priezjev and Troian 2004) observed a constant slip length at low shear rates and then a non-linear increase at higher shear rates. They interpreted this behavior by introducing the concept of a critical shear rate above which the wall can no longer impart additional momentum to the fluid. Their analyses of different length polymers indicated that slip length increases monotonically with chain length. (Khare et al. 1996) observed a trend of decreasing slip length with increasing shear rate (data reported in terms of slip velocity) which they validated by qualitative comparison to experimental studies. This group also evaluated the effect of chain length and found a non-linear relationship in which the effect of chain length was opposite for small and large polymers. The short chain behavior was attributed to molecular connectivity and the long chain behavior to chain packing. The trend of decreasing slip length with increasing shear rate is consistent with results reported by (Gupta et al. 1997) (data reported in terms of a slip parameter, S=1 – actual shear rate / apparent shear rate). That group utilized similar chain connectivity arguments to explain their results. (Jabbarzadeh et al. 1999) also reported slip in terms of the slip parameter S. However, they observe that slip decreases with increasing shear rate at lower shear rates, and then increases at very large shear rates. They attribute the low shear behavior to increasing fluid density which in turn pushes the fluid layers closer to the wall thereby reducing slip. The high shear behavior is explained as a washing of adsorbed fluid layers away from the walls.

The summary of different reported slip results shown here reveals that there is no consensus amongst the research groups. In addition, the different observed trends are interpreted

and utilized to make quite distinct predictions of slip behavior. Since the simulation tools employed by these research groups are so similar, it is unsettling to observe so many drastically different results. As will be discussed in the next paragraph, many groups have proposed reasons for discrepancies in reported results. However, it is likely the source of the inconsistency is not a single factor, but a combination of multiple effects.

One factor reported to greatly impact slip behavior is the interaction strength between the wall and fluid particles. Both (Jabbarzadeh et al. 1999) and (Manias et al. 1996) observe using molecular simulation that the degree of slip decreases with increasing wall-fluid interaction strength. This behavior is confirmed experimentally by (Leger 2003). (Jabbarzadeh et al. 1999) also observe, that for flexible wall models, slip increases with wall stiffness. Analyses of the effect of polymer chain length are reported by (Priezjev and Troian 2004) and (Khare et al. 1996). However, (Priezjev and Troian 2004) observe that slip length increases monotonically with chain length while (Khare et al. 1996) find a non-linear relationship in which the effect of chain length is opposite for short and long polymers. Surface roughness is also found to have a significant effect on slip by groups including (Jabbarzadeh et al. 1999) and (Priezjev and Troian 2005).

A less frequently investigated parameter is the channel width. The typical approach to exploring a range of shear rates is to vary the wall speed at a constant channel width. However, this approach cannot be used to capture the specific effect of the channel width. It is likely that channel width does have an effect based on the findings of (Lauga and Stone 2003) who observed that slip length scales with channel width. Because the shear rate is varied in the author's simulation by varying both wall speed and channel width, it is possible to investigate the

effect of both. It is observed that the channel width plays a significant role in slip behavior. For example, at a range of channel widths and two different wall speeds corresponding to a constant shear rate of  $\dot{\gamma} = 0.0625 \pm 2.8$ , the slip length varies by 44.4 %. This suggests that setting the shear rate does not uniquely fix the slip length. This is consistent with experimentally observed slip behavior. In fact, several groups, including (Cottin-Bizonne et al. 2002) and (Leger 2003), report that they observe no shear rate - slip length dependence.

It should be noted that significant inconsistency is also found in slip behavior obtained from experimental studies. (Cottin-Bizonne et al. 2002) compare the results from several such studies and find that slip lengths can vary by orders of magnitude. In their review paper on experimental slip measurements, (Huang et al. 2006) conclude that small differences in technique may explain variation of results.

## 9.3 Slip Length Scaled by System Size

The effect of channel width on slip can be pursued further by analysis of scaling. Typically, slip results from molecular simulation are normalized by the atomic length and time scales. However, in a comparative study of physical (as opposed to MD simulation) pressuredriven Poiseuille flow of mostly non-polymeric fluids, (Lauga and Stone 2003) find that slip length scales with system size. In that work, it as found that measured data spanned "large variations in the typical system size (more than 5 orders of magnitude in pipe radius or channel width), typical shear strain rates (4 orders of magnitude), typical values for the wall slip velocity (almost 6 orders of magnitude), and effective slip lengths (more than 4 orders of magnitude)." Despite this wide ranging span, "the variation in the dimensionless slip length  $\lambda_{eff}/R$ , where *R* is the characteristic channel dimension, is seen to be small; there is only a ration of 40 between its maximum and minimum values." (Lauga and Stone 2003) use  $\lambda_{eff}$  to refer to the slip length, but except for the quote above, the designation  $L_S$  will be used here. The author's MD simulations of Couette flow have been used to collect data simulation to that of (Lauga and Stone 2003). The data has been normalized by the system size, which in this case refers to the width of the channel and the speed of one wall. Table 9-2 shows the range of shear rates and slip lengths normalized in the conventional way using the molecular length and time scales compared to the same range normalized by the channel width.

Table 9-2: When non-dimensionalized with respect to molecular-scale parameters, shear rate and slip length vary by 3 and 2 orders of magnitude, respectively. However, as shown in the last two rows, when non-dimensionalized by channel width, their range of variations is reduced to one order of magnitude.

	Minimum	Maximum	Max / Min
<i>γ</i> τ	0.001	3.227	3227
$L_s / \sigma$	0.533	63.00	118
γh/U	0.320	1.638	24
$L_{s}/h$	0.110	2.625	11

Here it can be observed that using the typical atomic scale non-dimensionalization, shear rates vary by approximately 3 orders of magnitude and slip length varies by 2 orders of magnitude. The slip length, non-dimensionalized with respect to system size,  $L_s / h$ , varies only by a factor of 11. Comparison of the physical data of (Lauga and Stone 2003) with the author's simulation data reveals that, for both sets of data, scaling with system size leads to a compression of the range of values for the slip length. (Lauga and Stone 2003) suggest that the system-dependent

scaling may arise from nanobubbles arrayed at the wall. This supposition is reasonable and is supported by visual observations such that those reported by (Tyrrell and Attard 2001). But since there are no nanobubbles in the MD simulations, this suggests that the slip length scaling with system size may have another origin.

### 9.4 Location of Slip

Another unresolved question about slip is the location at which it occurs. That is, does slip occur between the wall and the first fluid layer, between two adjacent fluid layers, or at multiple locations. Consider that a measurement of shear rate and an independent measurement of slip speed are taken. For example, instead of determining the slip speed from the velocity profile extrapolated from the center of the channel to the wall, the average speed of the particles instantaneously near the wall was determined from  $v_s = U - \frac{1}{N} \sum_{i=1}^{N} \dot{x}_i(t)$  where the average is taken over the i = 1...N molecules which are adjacent to the wall. In physical experiments, it is also possible to measure the velocity close to the wall, and the nearness at which measurements can be taken is shrinking as experimental techniques improve. A recent example of such an experiment was reported by (Huang et al. 2006). Slip length can be calculated directly from measured slip speed as opposed to an extrapolation of the shear rate. To differentiate between these two calculation methods, the slip length obtained from the measured slip velocity will be denoted  $L_{s}^{'}$  . Conceptually, the relationship between the two definitions of slip length is illustrated as the left image in Figure 9-4.



Figure 9-4: Left – Conceptual diagram of the relationship between the slip length  $L_s$  calculated using the extrapolated shear rate, and  $L'_s$  calculated from the velocity of the fluid layer a discrete distance, d, from the wall. Right -  $L_s$  (filled diamonds) and  $L'_s$  (open diamonds) as functions of the inverse of shear rate all normalized by the system scale at a wall speed of 5.99  $\sqrt{\varepsilon/m}$ .

Based on this figure, it seems logical that  $L_s$  will be greater than  $L_s$  and that the difference between these two values will correspond to the distance from the wall to the first fluid layer. Both  $L_s$  and  $L_s$  were calculated from the author's simulations. The right image in Figure 9-4 shows a comparison of the two normalized by the system scale at a single wall speed. It can be observed that the slip length calculated from the simulated slip speeds does not trivially reflect the definition of slip speed. Rather it reveals to what extent the assumptions underlying the definition are met. If, for example, slip occurred a distance *d* from the wall, the slip speed would be  $v_s' = U - 1/2 \dot{\gamma} (h - d)$ . Using this expression we can solve for the *d* in terms of the shear rate and slip speed measured from the simulation. It is found that, for the wall speed illustrated in Figure 9-4, the distance from the wall at which slip occurs is relatively constant with a value of  $d = 1.69\sigma \pm 0.13$ . This is comparable to the location of the first fluid layer indicating that slip occurs between the first fluid layer and the wall. These observations are consistent with the displacement of the  $L'_s$  line upward from the  $L_s$  line in right-hand image of Figure 9-4 by approximately d/h.

The location of slip was investigated by (Manias et al. 1996) using MD simulation. They found that for weakly physisorbing surfaces ( $\varepsilon_{wall-fluid} = \varepsilon_{fluid-fluid}$ ) slip occurred only at the wall under any shear rate. However, for strongly physisorbing surfaces ( $\varepsilon_{wall-fluid} = 2\varepsilon_{fluid-fluid}$ ), slip behavior was dependant on shear rate. At low shear rates, there was no evident slip. But at high shear rates, there was slip both at the wall and between fluid layers. In the later case, the magnitude of the interlayer slip was significantly greater than that at the wall. The wall-fluid interaction strength in our simulations is smaller than the weakly physisorbing surfaces used by (Manias et al. 1996). Therefore, the observation made here that the slip occurs entirely in the first fluid layer is consistent with location expected based on the trends reported by (Manias et al. 1996).

Another means of investigating the location of slip is by comparison of the rate of momentum transfer at a wall-fluid interface to a fluid-fluid interface. Momentum transfer can be quantified by the discrete fluid-fluid,  $\eta_{ff}$ , and wall-fluid,  $\eta_{wf}$ , friction coefficients (Lichter et al. 2004). The discrete fluid-fluid friction coefficient is related to the bulk viscosity of the fluid by the atomic length scale (i.e.  $\eta_{ff} = \eta_{Bulk} \sigma$ ). The discrete friction coefficient between the fluid and the wall is related to the effective wall-fluid friction by the square of the atomic length scale

 $(\eta_{wf} = f_{wf}^{eff} \sigma^2)$ . The effective friction is the proportionality constant between the shear stress and the slip velocity.

The relationship between  $\eta_{gf}$  and  $\eta_{wf}$  can be investigated using the value of the bulk viscosity to obtain fluid-fluid friction, and shear stresses from molecular simulation to calculate the wall-fluid friction. The authors' extracted shear stress data from molecular dynamics simulations of n-decane fluid run at wall speeds of 10, 50, 100, and 1000 m/s and wall separations between 1.0 and 3.0 nm. The average value of the discrete wall-fluid friction coefficient was found to be  $\eta_{wf} = 3.55e-14$  kg/s. The bulk viscosity of n-decane at the simulation temperature of 300 K is 0.92 cP which corresponds to a discrete fluid-fluid friction coefficient of 3.62e-13 kg/s. Therefore, the fluid-fluid friction coefficient is one order of magnitude larger than that of the wall-fluid. This suggests that slip at the wall is larger than that between fluid layers.

Wall-fluid friction coefficient can also be estimated as a function of the fluid particle mass, *m*, the characteristic time,  $\tau$ , and a constant,  $\alpha$ , which represents the fraction of molecules thermalized by the wall (Sokhan et al. 2002). This expression is

$$\eta_{wf} = \frac{m}{\tau} \left( \frac{2\alpha}{2 - \alpha} \right) \tag{9.1}$$

The value of  $\alpha$  can be estimated using Maxwell's theory of slip which relates the distribution function of fluid velocity in the direction of mean flow before and after a collision with the wall. For Poiseuille flow of methane through flexible graphite walls,  $\alpha$  was found to be 0.023 (Sokhan et al. 2001). Using Equation 9.1 with the mass and time parameters given in that research, the wall-fluid friction coefficient is 3.14e-16 kg/s. The shear viscosity of methane subject to the above mentioned Poiseuille flow was reported as 5.3e-5 kg/m/s. This corresponds to a discrete fluid-fluid friction coefficient of 1.91e-4 kg/s. Therefore, in this case, the wall-fluid friction coefficient is 12 orders of magnitude larger than the fluid-fluid friction coefficient suggesting that all significant slip occurs at the wall. This approach is based on Maxwell's theory which is applicable only to a gas fluid. However, it is still interesting to evaluate the predicted friction coefficient relationships and corresponding suggested slip location.

## 9.5 Relating Slip to Solvation Pressure

As was shown in the Solvation Pressure chapter of this dissertation, the pressure perpendicular to the confining wall varies periodically with variable channel width. As discussed in that chapter, this oscillatory dependency arises due to the finite size of the fluid molecules, in which additional fluid "layers" are added only after discrete changes in channel width. A similar periodicity can be observed in the behavior of slip magnitude. This consistency is illustrated in Figure 9-5.



Figure 9-5: The slip length,  $L_s$ , and the solvation pressure,  $P_s$ , for different channel widths, *h*. The shaded bars are used to highlight periodicity as *h* is varied.

This figure demonstrates that behavior of slip length with variable channel width is consistent with that of solvation pressure.

The relationship between slip and solvation pressure has been quantitatively developed based on a treatment of slip as a rate process. Consider an equilibrium state  $G^0$  and a transition state  $G^+$  where  $G = \Theta + PV - TS$  is the Gibbs free energy. The flux rate from one state to the other is given by (Glasstone et al. 1941; Hanggi et al. 1990),  $k \propto \exp(-\Delta G^+ / (k_B T))$ , where  $\Delta G^+ = G^+ - G^0$ ,  $k_B$  is Boltzmann's constant, and T is temperature. If we assume that slip occurs through a rate process, namely  $v_s \propto k$ , then  $v_s(P)/v_s(P_0) \propto \exp[-(\Delta G^+ (P) - \Delta G^+ (P_0))/(k_B T)]$ , where  $P_0$  is a conveniently chosen reference solvation pressure. For a given wall speed, as the channel height is varied, we assume that the adiabatic component  $\Theta$  and the entropic term *TS* are constant, so we are left with

$$\frac{v_s(P_s)}{v_s(P_0)} = \exp\left[-\frac{(P_s - P_0)\Delta V^+}{k_B T}\right]$$
(9.2)

where  $\Delta V^+$  is the change of volume between the transition state and the equilibrium state. The temperature and solvation pressure are measured for each channel height from our simulation. After fitting a value for  $\Delta V^+$  (see below), the prediction using Equation 9.2 can be compared with the slip length data measured from our MD simulation as illustrated in Figure 9-6.



Figure 9-6: Comparison of slip length measured from our MD simulation to the value predicted using Equation 9.2 and converted to slip length using  $L_S = v_S / \dot{\gamma}$ . Here, f = 0.10 was fit to the data.

Equation 9.2 does reasonably well in matching both the amplitude and phase of the oscillatory variations in slip length.

A physical scenario can be ascribed to this rate process. With no applied shear, liquid molecules are most stable in the valleys of potential energy located between the solid lattice sites (Steele 1973). When shear is applied, liquid molecules move from one equilibrium site (valley) to another, needing to cross a pass of higher energy. The highest energy encountered is assigned

 $G^+$  and that in the equilibrium state  $G^0$ . The downstream hopping of a liquid molecule from one lattice site to another is equivalent to the upstream hopping of a vacancy: as a molecule hops into an unoccupied downstream site, its upstream initial position becomes vacated. The slip speed  $v_s$  is given by the mean number of vacancies times their mean rate k of hopping times the length per hop. We assume that the number of vacancies is at most weakly dependent on shear rate (Lichter et al. 2004), and so, as assumed above, find that  $v_s \propto k$ . The change in volume can now be estimated as follows. Following (Glasstone et al. 1941), we consider that the volume of the vacancy in the transition state is smaller than that in the equilibrium state, hence the negative sign in  $\Delta V^+ = -f(4\pi/3)\sigma^3$  where  $f \leq 0$  and  $\sigma$  is the Lennard-Jones size parameter for the wall-fluid interactions.

Evidence for slip as a rate process is also found in the literature. A recent study presents slip length as a function of temperature (Guo et al. 2005). Under the assumption that the shear rate in their Couette flow does not change appreciably as temperature is varied, we find that their data fits the expected exponential form of a rate process as illustrated in Figure 9-7.



Figure 9-7: The MD data of (Guo et al. 2005) (symbols) for two liquid densities. For a rate process,  $L_s \propto \exp(B/T^*)$ . *T*\* is the reduced temperature as defined by (Guo et al. 2005), and we find B = 1.44 (0.92) for the upper (lower) curve with  $R^2 = 0.9926$  (0.9960).

The formulation of (Kramers 1940) is expressly concerned with rate processes in solution. Kramers shows that rate is proportional to the bulk viscosity. Using molecular dynamics simulations, the slip of polymer solutions with a range of viscosities is reported in (Priezjev and Troian 2004). This data as well as that from physical experiments using sucrose solutions of different viscosities (Craig et al. 2001) both show the predicted linear dependence on viscosity, as illustrated in



Figure 9-8: Slip length  $L_s$  shows the predicted linear dependence on viscosity  $\eta$ . For the MD data for polymeric solutions (Priezjev and Troian 2004) (squares),  $\eta$  and  $L_s$  are the nondimensional viscosity x 10 and slip length respectively as defined in (Priezjev and Troian 2004). The physical experiments of (Craig et al. 2001) use sucrose solutions at a low (7300 nm/s: closed circles) and high(11900 nm/s: open circles) rates of driving. For their data, the values along the abscissa are in cP, the slip length is in nm, and error bars are from (Craig et al. 2001). The coefficients of determination, from top to bottom, are  $R^2 = 0.9967$ , 0.9686, 0.9996.

It may be seen as surprising that polymer slip is due to vacancies. However, the slip length vs. shear rate curves for the polymer solutions presented in Figure 3 of (Priezjev and Troian 2004) collapse onto a single curve with single monomer data, as shown in Figure 4 of (Priezjev and Troian 2004). The analytic form of this curve is, furthermore, identical to that found for simple liquids (Thompson and Troian 1997). The authors of (Priezjev and Troian 2004) "support the view that [slip behavior]...for simple fluid systems [are] more generally applicable to polymeric systems." It seems then, not unreasonable that the slip mechanism should similarly encompass both simple and polymeric liquids. Less direct evidence is also provided by x-ray reflectivity, in which sheared polymers appear to disentangle and lie down along the substrate (Yu et al. 2003), as suggested by molecular layering experiments (Heslot et al. 1989; De Coninck et al. 1995).

Following LeChatelier's principle, high pressures can accelerate the rate to the transition state. Treating slip as a rate process incorporates the work done by the solvation pressure. This treatment allows us to make sense out of what otherwise seem to be contradictory observations. On the one hand, it is expected that since the potential due to the solid falls off rapidly with distance above the solid, liquid molecules lying further from the solid would slip more easily. At fixed solvation pressure, this is a correct observation. However, channels of varying height filled from the same reservoir will vary in their solvation pressure, leading to flows with different amounts of slip. In comparing these cases, the work done by the liquid can lead to the opposite result of the constant density case, in which proximity to the solid facilitates slip.

In conclusion, a consequence of the discreteness of molecules is that the liquid molecules have energetically preferred configurations. In order for slip to occur, the liquid molecules must leave these stable sites. We have shown that in addition to overcoming the adiabatic solid potential, there is another component to the energy landscape, namely the work supplied by the solvation pressure of the liquid environment. The effects of solvation pressure may be quantitatively accounted for by treating slip as a rate process. The physical process which accommodates the data is one in which liquid molecules hop downstream along the liquidsolid interface, or equivalently vacancies hop upstream.

# 9.6 Conclusions

In this chapter, molecular dynamics simulation was use to investigate several different aspects of slip behavior. The following is a summary of the findings:

- Comparison of slip behavior reported from literature studies utilizing molecular simulation of polymer fluids subject to Couette flow reveals that significant variation in both the magnitude of slip and its relationship to shear rate. In addition, the authors of the reviewed articles interpret and explain their results using very different arguments.
- Scaling slip with system size (as opposed to molecular length and time scales) leads to a compression of the range of slip and shear rate values.
- Analyses of the wall-fluid friction as well as alternate means of calculating slip indicate that slip in these simulations occurs entirely in the first fluid layer.
- A relationship between slip magnitude and solvation pressure is identified that can be understood if slip is viewed as a rate process. Additional support for the concept of slip as a rate process is obtained using slip dependence on temperature and viscosity obtained from the literature.

Each of these provides insight into not only our ability to characterize slip behavior but also to understand slip on the molecular scale.

# Chapter 10 Thin Film Viscosity

### 10.1 Background

The last of the unique thin film properties to be discussed is viscosity. Characterization of the viscosity of thin films has been the focus of many research efforts because thin film viscosity may not adhere to behavior predicted using continuum models. Two viscosity phenomena that are particularly significant in thin films under shear will be investigated here. These are shear thinning and oscillation with film thickness. Shear thinning, the decrease of viscosity with increasing shear rate, is not specific to thin films. However, it is particularly important in thin film rheology studies because thin film lubricants are subject to large shear rates (above the limit at which shear thinning occurs) even under moderate operating speeds. Shear thinning has been extensively investigated in larger-scale liquids using experimental techniques (Bair 2001; Bair et al. 2005). However, in nano-confined fluids, shear thinning behavior is primarily investigated using molecular dynamics simulation (Thompson and Robbins 1990; Jabbarzadeh et al. 1998; McCabe et al. 2001; Kioupis and Maginn 2002). Although the mechanism behind shear thinning on different length scales may not be the same, it has been found to follow consistent, length scale-independent behavior using the time temperature superposition principle (Bair et al. 2002).

Molecular simulation is utilized to characterize viscosity at a range of applied or actual shear rates. In these simulations, the shear rate is usually varied by modulating the wall speed and maintaining constant film thickness. However, the viscosity predicted at a given shear rate predicted using this approach may not be applicable to a different combination of film thickness and wall speed that correspond to the same shear rate. One reason for this is that viscosity has been found to oscillate with variable film thickness in ultra thin films (Wang and Fichthorn 2002). Constant film thickness studies cannot capture this effect. This research characterizes thin film viscosity using molecular simulations run at both variable wall speed and variable film thickness. This approach enables evaluation of the effect of both film thickness and shear rate (i.e. shear thinning) and the development of a composite viscosity model that incorporates the effects of both shear thinning and oscillation with film thickness. Some of the content of this chapter is also available in (Martini et al. 2006).

### **10.2 Results and Analysis**

### **10.2.1 Calculation Method**

Viscosity was calculated from MD simulation as the ratio of shear stress,  $\tau_{xz}$ , to shear strain rate,  $\dot{\gamma}$ .

$$\eta_{xz}^{MD} = \frac{\left\langle \tau_{xz} \right\rangle}{\dot{\gamma}} \tag{10.1}$$

The shear stress for each set of operating conditions was averaged over several simulations run to a total duration of between 1 and 2 ns (slower shear rates run longer to improve statistical accuracy).

Researchers use several different methods for calculating shear stress from MD simulation. One of the most frequently used expressions is the average shear force of the lubricant atoms on the wall atoms divided by the area of the walls.

$$\tau_{xz} = \sum_{i}^{N_{wall}} \sum_{j}^{N_{Flaid}} F_{x}^{ij} / A$$
(10.2)

This method of stress calculation has been found to yield the same results as the Method of Planes (Todd et al. 1995) if the plane is chosen to be at the position of the walls (Varnik et al. 2000; Zhang et al. 2001). Another popular method is the Irving-Kirkwood relationship. The Irving-Kirkwood expression and Equation 10.2 were found to yield similar results both in this research and others (Jabbarzadeh et al. 1998). Therefore, to improve the accuracy of results, both methods were used and the results averaged.

The shear strain,  $\dot{\gamma}$ , was considered to be the applied shear rate (i.e. wall speed divided by wall separation). Viscosity calculated using the applied shear rate is often termed the effective viscosity. Effective viscosity assumes that the velocity of the fluid layer next to the walls is the same as that of the wall (i.e. no-slip). It has been found that this assumption is not always applicable to thin films under shear. However, effective viscosity is still frequently used as a measure of the viscous behavior of thin films (Thompson et al. 1992; Hu and Granick 1998; Jabbarzadeh et al. 1998; Balasundaram et al. 1999). Use of effective viscosity is common not only because it is readily obtained from MD simulation, but because its calculation method is consistent with that used in viscosity measurements taken using a surface force apparatus (Zhang et al. 2001). Effective viscosity was also used in this research.

### **10.2.2 Molecular Simulation Results**

Simulations were run at applied shear rates of between  $6.7 \times 10^9$  and  $3.3 \times 10^{11}$  l/s. This range was attained by running simulations at both variable film thickness (0.6 to 3.0 nm) and

variable wall speeds (1 to 100 m/s). The resultant viscosity is illustrated as a function of shear rate in Figure 10-1 and of film thickness in Figure 10-2.



Figure 10-1: Molecular dynamics viscosity results at wall speeds of 1, 5, and 10 m/s as a function of shear rate.



Figure 10-2: Molecular dynamics viscosity results at three different walls speeds as a function of film thickness. Exact data points connected by a smooth curve to illustrate oscillatory behavior.

Two primary trends can be observed from these results. First, the viscosity decreases with increasing shear rate. And second, the viscosity oscillates as a function of film thickness. Decreasing viscosity with increasing shear, or shear thinning, is a well researched phenomenon. However, oscillatory behavior is typically not observed in these studies. This may be attributed to the fact that studies of thin film behavior are often performed on cases where the film thickness is either not changed, or the difference between film thicknesses in consecutive test is much larger than the 0.1 nm used in this research. In either of these cases, the high frequency

oscillation observed in Figure 10-2 may not be observable. Both the shear thinning and oscillatory effects will be analyzed and then incorporated into a composite thin film viscosity model.

The phenomenon of enhanced viscosity, or solidification, in very thin films was not observed in this research. Solidification has been observed both experimentally (Hu et al. 1991; Smeeth et al. 1996) and using MD simulation (Hu et al. 1998; Jeng et al. 2003). However, solidification is typically exhibited in unmoving or slowly moving fluids. Fluids under large, continuous shear, such as those studied in this research, are not expected to exhibit solidification (Granick 1991; Hu and Granick 1998).

## 10.2.3 Shear Thinning

The effect of shear rate on viscosity is often described using a power law relationship. One such model used frequently is the Carreau equation (Ponton et al. 1998; Bair 2002; Kioupis and Maginn 2002).

$$\eta^{ShearThinning}(\dot{\gamma}) = \frac{\eta_0}{\left[1 + (\dot{\gamma} / \dot{\gamma}_c)^2\right]^{n/2}}$$
(10.3)

In this expression,  $\eta_0$  is the viscosity of the fluid subject to zero or low shear,  $\dot{\gamma}_c$  is the critical shear rate above which shear thinning occurs, and *n* is the slope of the  $\log \dot{\gamma} - \log \eta(\dot{\gamma})$  curve in the shear thinning region. In the present simulation, the fluid was allowed to heat up and therefore the effect of temperature must also be considered. Both the zero shear viscosity and the critical shear rate have been found to be functions of temperature (Ponton et al. 1998). Although an exact expression relating critical shear rate to temperature is not available, it has been observed that increasing temperature corresponds to increasing the critical shear rate

(Ponton et al. 1998). The relationship between zero shear viscosity and temperature is better understood, and there are several empirical and theoretical expressions available. One of the most accurate of these is the Vogel equation (Stachowiak and Batchelor 2001).

$$\eta_0 = b \exp(c/T - d)$$
(10.4)

In this expression, *b*, *c*, and *d* are fluid dependant, empirical constants. For bulk n-decane, experimental viscosity-temperature data (Lemmon et al. 2005) can be used to obtain b=0.03 cP, c=787 K, and d=69 K. The simulations reported here were run at three different wall speeds which resulted in three different average fluid temperatures. The Vogel equation was used to calculate the corresponding zero shear viscosities of 0.92 cP at 300 K, 0.83 cP at 306 K, and 0.71 cP at 318 K.

Since the fluid temperature was different at each wall speed, and both the zero shear viscosity and the critical shear rate are functions of that temperature, the Carreau shear thinning model must be fit to the simulation data at each wall speed independently. This approach was used to obtain an average value for the exponent, n, and to determine the relationship between critical shear rate and temperature. The resultant fit for each wall speed is illustrated in Figure 10-3.



Figure 10-3: Viscosity as a function of shear rate at three wall speeds. Exact data points (hollow shapes) fit with the Carreau shear thinning model (solid line). Temperaturedependent zero shear viscosity (horizontal dashed lines) and critical shear rate (vertical arrow) indicated.

It was found that the critical shear rate does in fact increase with temperature. The critical shear rate increased asymptotically towards  $\dot{\gamma}_C^{\text{max}} = 1.4 \times 10^{11} \text{ 1/s}.$ 

The shear thinning exponent, *n*, has been found to be relatively constant by many different researchers using a variety of simulation and experimental techniques. In addition, it has been found to be independent of temperature (Ponton et al. 1998). Typically, its value is reported to be between 1/2 and 1. Larger values are found to correspond to extreme conditions such as high load, small film thickness, or large shear rate (Hu and Granick 1998). The average value calculated from the three wall speeds considered in the present work was  $0.91 \pm 0.10$ . Other MD simulation studies of n-decane under wall imposed shear reported a value of 0.56 (Balasundaram et al. 1999). Differences in reported values for this exponent can be attributed to the effect of simulation parameters such as wall surface corrugation, wall fluid strength, and applied normal load. In addition, the shear rate was varied in the present research by changing the film thickness at constant wall speed. This differs from the approach used by other researchers in which the shear rate was modulated by varying the wall speed at constant film thickness (Balasundaram et al. 1999).

### **10.2.4 Oscillation with Film Thickness**

As illustrated in Figure 10-2, viscosity was observed to oscillate as a function of film thickness where the frequency of oscillation is independent of wall speed. Viscosity has been found to oscillate with film thickness in thin films by researchers studying fluids in equilibrium (Wang and Fichthorn 2002). In that research, the oscillatory viscosity behavior was partially validated using comparison to the behavior of solvation pressure. Solvation pressure,  $P_S$ , arises from the force that acts between two walls with a very thin layer of fluid separating them as
discussed in the Solvation Pressure section. The solvation pressure and viscosity as functions of film thickness from the 100 m/s wall speed simulation are illustrated in Figure 10-4.



Figure 10-4: Solvation pressure (hollow circles) and viscosity (solid squares) as functions of film thickness. Consistent frequency of oscillation illustrated by shaded bars.

It can be observed that the frequency of oscillation is approximately the same for the viscosity and solvation pressure. This suggests that the viscosity oscillation has a physical origin. The relationship between solvation pressure and viscosity illustrated for this wall speed case is representative of all wall speeds evaluated.

The relationship between film thickness and solvation pressure has been modeled using a sinusoidal expression (Abd-AlSamieh and Rahnejat 2001).

$$p_{zz}(h) = -A_p e^{-h/r} \cos\left(\frac{2\pi h}{\lambda}\right)$$
(10.5)

In this expression,  $A_p$ , r, and  $\lambda$  are constants that can be fit from experimental or simulation data. Physically, these constants represent the amplitude,  $A_p$ , the rate of decay, r, and the oscillation wavelength,  $\lambda$ . Experimental research on octamethylcyclotetrasiloxane produced values for these constants as  $A_p=172$  MPa and  $r=\lambda=1$  nm (Abd-AlSamieh and Rahnejat 2001). In this research on n-decane, these constants were found to be  $A_p=325$  MPa, r=1.45 nm, and  $\lambda=0.37$  nm. All of these constants were found by other researchers (Horn and Isrealachvili 1981) and in the present work to be largely independent of temperature. The comparison between solvation pressure and viscosity in Figure 10-4 indicates that the wavelength and decay rate of the viscosity and solvation pressure curves are approximately the same. Therefore, it is expected that the oscillation in viscosity can be described using a sinusoidal expression similar to that for solvation pressure where only the amplitude is different. This expression describing the oscillation of viscosity with film thickness is

$$\eta^{Oscillation}(h) = -A_{\eta} e^{-h/r} \cos\left(\frac{2\pi h}{\lambda}\right)$$
(10.6)

Here, the constants r and  $\lambda$  are the same as in the expression for solvation pressure (i.e. the decay rate and wavelength are the same). But the amplitude,  $A_{\eta}$ , is different. The value of the viscosity amplitude was found to be  $A_{\eta}$ =0.084 *cP*. The accuracy of this fit to the molecular simulation data will be evaluated in the next section as part of the analysis of the composite thin film viscosity model.

### 10.2.5 Composite Viscosity Model

In the previous two sections, viscosity was characterized in terms of oscillation with film thickness and shear thinning separately. A composite viscosity model would contain contributions from both. A proposed expression of this form is

$$\eta(\dot{\gamma}, h, T) = \frac{\eta_0(T)}{\left[1 + \left(\dot{\gamma} / \dot{\gamma}_c(T)\right)^2\right]^{n/2}} - A_\eta e^{-h/r} \cos\left(\frac{2\pi h}{\lambda}\right)$$
(10.7)

The values of the constants corresponding to the simulation parameters used in this research are summarized in Table 10-1.

 Table 10-1: Composite thin film viscosity model constants, physical meaning, and either approximate value or functional form.

Constant	Physical Meaning	Value/Function	Units
ηο	Zero shear viscosity	Vogel: b exp(c / (T-d)) b = 0.03 cP c = 787 K d = 69 K	сP
ý <sub>c</sub>	Critical shear rate	Asymptotic: $y_c \in (y_c^{max})$ $y_c^{max} = 1.4 \times 10^{11}$ 1/s	1/s
n	Shear thinning exponent	0.91	-
$A_{\eta}$	Oscillation amplitude	0.069	сP
r	Oscillation decay rate	1.29	nm
Л	Oscillation wavelength	0.37	nm

Using Equation 10.6 with the constants reported in Table 10-1, the current simulation results can be predicted as a function of shear rate and film thickness. The exact simulation data points are compared to the composite thin film viscosity model in Figure 10-5.



Figure 10-5: Comparison of the simulation results (solid squares connected by dotted line) with viscosity predicted by the composite thin film viscosity model (solid line).

The overall RMS measure of fit accuracy is 0.85. The inaccuracy is due in part to the low shear data. It is expected that shear stress (and therefore viscosity) calculations from non equilibrium MD simulations are less accurate at lower shear rates.

### 10.2.6 Conclusions

Molecular simulation was used to characterize viscosity in a confined fluid subject to high shear rates. Simulations were performed at variable wall speed and film thickness such that the effects of both parameters could be evaluated. It was found that the viscosity of thin films is subject to both shear thinning and oscillation with film thickness. A composite model was developed that incorporated both effects.

# Chapter 11 Future Work

## 11.1 Background

Chapters 7 - 10 of this dissertation discussed four of the primary factors that distinguish confined fluids from their bulk counterparts. These are density, solvation pressure, interface slip, and viscosity. The first step towards integrating these behaviors into a thin film lubricated interface simulation is to identify where the unique thin film behavior may have an impact on continuum models that are traditionally used to describe lubricated interface behavior.

A mixed elastohydrodynamic lubricated (EHL) interface is subject to four primary phenomena: Lubricant flow through the interface, elastic deformation of the solid bodies, material wear, and the change of lubricant properties with operating conditions. A simulation of a mixed EHL system incorporates models of these phenomena. Some of the models were introduced in Chapter 5. Also, a detailed description of the models and their implementation into numerical solution is available in (Hu and Zhu 2000; Zhu and Hu 2001; Zhu and Hu 2001). The key equations will be presented briefly here for reference.

• Lubricant flow is typically described by the Reynolds equation. A commonly reported, transient form of this expression is

$$\frac{\partial}{\partial x} \left( \frac{\rho h^3}{12 \eta} \frac{\partial p}{\partial x} \right) + \frac{\partial}{\partial y} \left( \frac{\rho h^3}{12 \eta} \frac{\partial p}{\partial y} \right) = U \frac{\partial (\rho h)}{\partial x} + \frac{\partial (\rho h)}{\partial t}$$
(11.1)

where, h is film thickness,  $\rho$  is density, p is hydrodynamic pressure, and  $\eta$  is viscosity.

• Elasticity of the contacting solids is modeled based on deformation due to a normal pressure distribution as mathematically described in Equation 11.2 where *E*' is the elastic modulus.

$$V(x, y, t) = \frac{2}{\pi E'} \iint_{\Omega} \frac{p(\xi, \varsigma)}{\sqrt{(x - \xi)^2 + (y - \varsigma)^2}} d\xi d\varsigma$$
(11.2)

• Friction in at mixed EHL interface is the sum of hydrodynamic friction and contact friction. The hydrodynamic friction is calculated in hydrodynamically lubricated areas using Bair and Winer's non-Newtonian elastic-viscous fluid model.

$$\dot{\gamma} = \frac{\tau}{G_L} - \frac{\tau_L}{\eta} \ln \left( 1 - \frac{\tau}{\tau_L} \right) \tag{11.3}$$

where  $G_L$  is the limiting shear elastic modulus of lubricant, and  $\tau_L$  the limiting shear stress, which can be estimated empirically or experimentally. Friction in the contact areas is obtained using an experimentally estimated boundary lubrication coefficient of friction (typically between 0.08 and 0.12).

• Variations in viscosity with changing conditions in the interface are typically modeled in terms of pressure, temperature, and shear rate. The pressure dependence can be described by an exponential relationship such as the Barus equation.

$$\eta = \eta_0 \exp(\alpha p) \tag{11.4}$$

Models that describe the dependence of viscosity on temperature (e.g. Vogel equation) and shear rate (e.g. Carreau equation) were introduced in Chapter 10.

• The change of density with pressure can be modeled using the Dowson-Higginson expression.

$$\rho = \rho_0 \left( 1 + \frac{0.6 \times 10^{-9} \, p}{1 + 1.7 \times 10^{-9} \, p} \right) \tag{11.5}$$

• Wear of the solids in an interface can be described using many different, application specific models (Goryachev 1998). Here, the Archard wear law will be used as a representative model for wear rate, dW/dt.

$$\frac{dW}{dt} = k \frac{pU}{H} \tag{11.6}$$

In this expression, H is the material hardness, U is the speed, and k is a material and operating condition dependent wear coefficient.

Although there have been many different expressions proposed to model phenomena that occur in a mixed EHL interface, most equations contain the same parameters and, in most cases, are of the same form as Equations 11.1 - 11.6. Therefore, a preliminary evaluation of the potential impact of thin film behaviors can be performed using only these representative equations. In the next section, each thin film behavior will be analyzed individually in terms of overlap with expressions that describe mixed EHL behavior.

#### 11.2 Continuum-Molecular Overlap

#### 11.2.1 Density

It was observed in Chapter 7 that density in confined fluids exhibits two significant unique behaviors – formation of discrete layers near the confining walls and a decrease of the average density with decreasing film thickness. Both of these will potentially impact a thin film lubricated interface. The first, inhomogeneity of the density across the thickness, is contrary to one of the assumptions made in derivation of the commonly used form of the Reynolds equation (Equation 11.1), that the density is constant across the film. To resolve this issue, a density profile can be first characterized using molecular simulation in terms of the film thickness and molecular properties. Then the continuum assumption,  $\partial \rho / \partial z = 0$ , can be replaced with the characterization obtained from the simulation, and an alternative form of the Reynolds equation developed.

The second property of thin film density described in Chapter 7 is that the average density of a confined film may be less than the same fluid in the bulk. To integrate this effect into the EHL models, the bulk average density can be simply replaced by the lesser, thin film value. For example, this substitution can be made for the average density in fluid flow expressions describing the two directions parallel to the confining walls. The confined film average density can be obtained using the formulation based on excluded volume theory,  $\overline{\rho} = \rho_{bulk} (h - h_e)/h$ . The appropriate value of the excluded volume (or in this case excluded distance,  $h_e$ ) can be identified using molecular simulation. Then, for each discrete location in an

EHL interface, the average density can be calculated as a simple function of the film thickness at that location and, lastly, the results utilized in fluid flow calculation.

#### **11.2.2 Solvation Pressure**

A brief review of Equations 11.1, 11.2, 11.4, 11.5, and 11.6 reveals that pressure is a parameter in all of them and therefore plays an important roll in modeling of a lubricated interface. In Equations 11.1, 11.3, and 11.4 the pressure term is the hydrodynamic pressure in the fluid. These equations describe the fluid flow, change of lubricant viscosity with pressure, change of lubricant density with pressure, respectively. As was observed in Chapter 8, the magnitude of solvation pressure may become significant in thin films. If solvation pressure is on the same order of magnitude as the hydrodynamic pressure, then it may have to be incorporated in the expressions that describe lubricant flow, viscosity, and density in an interface. In this case, the load is supported by the lubricant through the combined effects of the hydrodynamic pressure,  $p_h$ , and the solvation pressure,  $p_s$ . Therefore the total pressure is  $p = p_h + p_s$ . This summation of pressures has been justified using Bernoulli's Principle of Superposition (Abd-AlSamieh and Rahnejat 2001). Incorporation of the solvation pressure into a fluid flow model has been done before (Matsuoka and Kato 1997; Abd-AlSamieh and Rahnejat 2001). In both cases, the solvation pressure was found to introduce fluctuations in the calculated pressure distribution that are most significant near the inlet and outlet of the interface. Additionally, it was found that calculations of average film thickness using a fluid flow expression that incorporates solvation pressure reflect experimental observations of thin film drainage experiments (Matsuoka and Kato 1997). In a numerical solution, the viscosity and density of the lubricant are adjusted each time step based on the changing fluid pressure. Therefore, if solvation pressure is introduced in the fluid flow equation, it will be also reflected in the models for lubricant density and viscosity.

In Equations 11.2 and 11.6 that describe elastic deformation and material wear (i.e. plastic deformation), respectively, the pressure term is due to either hydrodynamic or contact pressure. In areas of direct solid to solid contact, solvation pressure effect will not impact the elasticity or wear models. However, in areas where the solids are separated by a thin lubricating film, the pressure term may have to incorporate both hydrodynamic and solution pressures. As in the fluid flow equation, the pressure in the elasticity and wear equations is then  $p = p_h + p_s$  for thin film lubricated areas.

As described in Chapter 8, solvation pressure can be characterized in terms of molecular properties of the lubricant and wall, and the film thickness (referred to in Chapter 8 as channel width). Assuming that molecular characteristics do not vary, solvation pressure is then simply a function of film thickness. Local film thickness is a readily available parameter in a numerical EHL simulation. Therefore, the variation of solvation pressure with film thickness modeled using molecular simulation can be incorporated directly in an EHL simulation.

#### 11.2.3 Interface Slip

Interface slip, or the difference in velocity between a solid and the lubricant immediately next to it, was described in Chapter 9. As discussed in detail in that chapter, the magnitude of slip may become significant in thin films. In traditional continuum models, the "no slip" condition is frequently employed which assumes that the solid and adjacent liquid velocities are the same. This assumption is utilized in two places: As a boundary condition for solution of the

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fluid flow equation, and to calculate the fluid shear rate and corresponding hydrodynamic friction. First consider the boundary condition. The typical "no slip" fluid flow boundary condition can be expressed u(z = 0, h) = U where U is the wall speed. However, if the slip velocity,  $u_{slip}$ , is significant, it can be characterized from molecular simulation (or calculated from solvation pressure as described in Chapter 9), and its magnitude can be introduced directly as a boundary condition as  $u(z = 0, h) = U - u_{slip}$ . This approach has been employed in simulation of gas lubrication in a hard disk drive (Sun et al. 2002). In that work, it was found that introduction of slip into flow models results in a decrease of the pressure distribution and corresponding load-carrying capacity. In addition, the slip models showed good agreement with predictions made using the linearized Boltzmann equation (Sun et al. 2002).

Slip also impacts the fluid shear rate. In the "no slip" limit, the fluid shear rate is equal to the imposed shear rate, du/dz = 2U/h (for two walls moving in opposite directions with speed U). However, with a slip speed incorporated, this becomes  $du/dz = 2(U - u_{slip})/h$ . Based on this expression, if the slip speed is large, the actual fluid shear rate may be significantly less than the applied shear rate. Fluid shear rate may impact an EHL interface simulation through shear thinning (see section 11.3) or frictional heating. Hydrodynamic friction is a function of shear rate. Therefore, if the fluid shear rate is less than the applied shear rate, the hydrodynamic friction will be overestimated by Equation 11.3. Using an approach similar to that described for the fluid flow boundary condition, the slip velocity can be characterized using molecular simulation and then introduced into the frictional shear model. The result would be a friction model that is applicable to thin lubricating films.

#### 11.2.4 Thin Film Viscosity

Viscosity of the lubricant plays a critical role in models of fluid flow. In traditional EHL models, the viscosity of the lubricant in the interface is characterized in terms of the effects of pressure, temperature, and shear rate. However, in Chapter 10, viscosity was found to oscillate as a function of film thickness when the film is molecularly thin. It is well known that film thickness varies in an EHL interface. Therefore, in a thin film EHL interface, the variation of viscosity with film thickness may have to be incorporated into the model. Detailed analyses of the anticipated variation of viscosity due to film thickness in an interface will be presented in the next section.

#### 11.3 Variation of Viscosity in a Thin Film Interface

In Chapter 10, thin film viscosity was characterized using molecular simulation. A composite thin film viscosity model was developed from the simulation results that incorporated the effects of both shear thinning and oscillation with film thickness. This model is directly applicable to a thin film EHL interface in which both the wall speed and film thickness may vary. Here, the variation of viscosity in an EHL interface predicted using the composite thin film model will be evaluated. This analysis is performed using the film thickness and pressure distributions predicted by a continuum EHL simulation. Some of the content of this section is also available in (Martini et al. 2006).

#### 11.3.1 Modeled System

Recall from Chapter 10 that the composite thin film viscosity mode (Equation 10.7) predicted that shear thinning would become significant at shear rates above a critical value on the

order of  $10^9$  1/s and viscosity will oscillate with variable film thickness less than approximately 2.5 nm. Therefore, to evaluate the impact of this model on an EHL interface, the interface has to operate within this range of shear rates and film thicknesses. For this illustration, a simple case of point contact between ideally smooth surfaces. The operating conditions and material properties are summarized in Table 11-1.

Parameter	Symbol	Value	Units
Reduced Modulus	E'	117	GPa
Reduced Radius	R <sub>x</sub>	2	μm
Mean sliding speed	U	10 (0.1)	m/s (nm/ps)
Load	W	0.1	mN
Ambient Temperature	To	300	К

Table 11-1: Summary of the EHL simulation operating conditions and material properties.

This geometry can be viewed as an idealized single asperity interaction. The radius corresponds to the size of the smallest significant asperity and the applied load is the load on that asperity. The Hamrock-Dowson (Stachowiak and Batchelor 2001) predicted average and minimum film thickness values for this case are 1.7 nm and 2.7 nm respectively. These correspond to effective shear rates of  $5.9 \times 10^9$  and  $3.7 \times 10^9$  1/s. It is therefore expected that the composite thin film viscosity model will have an effect for a contact with film thickness and shear rates in these ranges.

#### **11.3.2 Interface Area Viscosity**

The EHL simulation was run initially without considering the effects of shear rate and film thickness on viscosity. Then, the wall speed and temperature input into the continuum simulation, and the output film thickness distribution across the interface were substituted into the composite thin film viscosity model (Equation 10.7) in order to predict the corresponding viscosity change. The interface area film thickness and corresponding predicted change in viscosity due to thin film effects are illustrated in Figure 11-1. The film thickness is normalized by the Hertz contact radius (137 nm) and the viscosity is normalized by the low shear, bulk viscosity of n-decane at 318 K ( $\eta_0$ =0.71 cP). Analyses of the film thickness are to decrease viscosity in the interface area.



Figure 11-1: Interface film thickness normalized by the Hertzian contact radius (top) and corresponding predicted change in viscosity due to shear rate and film thickness normalized by the bulk, low shear value (bottom). The direction of motion, *x*, is from left to right.

The predicted viscosity change due to shear rate and film thickness can be evaluated using two dimensional distributions across the interface centerlines. The film thickness and corresponding predicted change in viscosity along the x and y direction centerlines are illustrated in Figure 11-2.



Figure 11-2: x-direction (left) and y-direction (right) interface area centerline distributions of normalized film thickness (solid line) and normalized predicted thin film viscosity (dashed line).

The centerline viscosity distributions indicate that the most significant changes in viscosity due to shear rate and film thickness are expected to occur near the perimeter of the interface area. At these locations, both shear thinning (normalized viscosity less than one) and oscillation may occur. The largest predicted viscosity change was approximately a 50% decrease that was observed at the sides of the interface. However, the viscosity at the inlet area may be of more importance because it is this area that is critical in forming an EHL film (Stachowiak and Batchelor 2001). Therefore, changes in viscosity due to shear rate and film thickness at the inlet may have a significant effect on the overall EHL film thickness. For the operation conditions and material properties considered here, the composite thin film viscosity model predicts a viscosity decrease of approximately 15% as well as oscillatory behavior at the inlet. It is expected that these

changes, although small compared to the edge effects, will have the most significant impact on the EHL film.

#### **11.3.3 Numerical Integration Plan**

The next step is to integrate the composite thin film viscosity model into an EHL simulation. It is proposed that this be done with an approach similar to those typically used for developing non-Newtonian EHL models. Non-Newtonian EHL models integrate the effect of shear thinning into a traditional EHL model in order to develop a modified Reynolds equation. The details for one such integration can be found in another publication (Johnson et al. 1985). Only a brief description of the approach will be presented here. First, the rheological model is extended to two-dimensional vector form. Then, linear shear forces are expressed along the film thickness based on force balance. Next, the expressions for shear flow are integrated in accordance with the rheological constitutive equation. Applying speed boundary conditions, shear forces at the central layer in two directions are determined. And finally, new flow rate factors are calculated for the modified Reynolds equation. The composite (i.e. shear thinning and oscillation) viscosity model developed in this work will be integrated into the Revnolds equation using a similar approach. The primary difference is that the oscillatory behavior is a function of film thickness. Therefore, both film thickness and shear rate will have to be considered in the derivation of the modified Reynolds equation.

#### **11.4 Conclusions**

In this chapter, the potential overlaps between continuum models of an EHL interface and the unique behaviors of thin films were identified. Specifically, the effects of thin film density, solvation pressure, interface slip, and thin film viscosity on EHL phenomena of fluid flow, elastic deformation, material wear, and lubricant properties were evaluated. Identification of these overlaps is the first step towards ultimately integrating thin film characteristics into an EHL simulation. The next step to quantifying the potential impact of thin film behavior on an interface was illustrated using thin film viscosity as an example. The expected impact that this model would have on an EHL interface was evaluated using a continuum simulation.

# **Concluding Remarks**

In this dissertation, the problem of thin film lubrication was approached from two completely different directions – continuum lubricated contact modeling and atomistic simulation of thin film behavior. The motivation behind the work was to build a foundation for future development of thin film lubrication models. However, in the process, significant contributions were made to both the fields of continuum tribological modeling and molecular simulation-based characterization of thin film behavior.

First, a transient, 3D, analytical expression was formulated to describe thermoelastic displacement due to frictional heating and convection. The resultant model was incorporated into a numerical solution in order to investigate the effect of convection at an interface. Then, a contribution was made to the important area of stress modeling by development of a simplified model for rapid prediction of maximum subsurface stresses. The model utilized smooth surface approximations to estimate both the magnitude of the maximum stresses at the critical locations below the surface where they occur (i.e. near surface due to asperity interactions and further below due to the global shape of the contact). The usefulness of the model was also expanded by introduction of an enhancement which enables improved prediction of mixed EHL wear was evaluated by comparison of the model results to experimental trends reported in the literature. These comparisons were based on the evolution of the two surfaces, the film thickness, pressure, and subsurface stress distributions before and after wear, and the phases that the interface undergoes during the wear process.

Contributions to thin film research were made possible through the enhancement of an existing molecular dynamics simulation to incorporate the critical properties of a lubricated interface. Once validated, the simulation was used as a tool to probe the behavior of thin films under shear. The density of a confined fluid was characterized in terms of the formation of atomistic-scale layers next to the confining walls and an overall decrease of the average density attributable to excluded volume effects. Solvation pressure was measured from simulation and found to oscillate with channel width. Careful analysis of this behavior and the structural properties of the fluid atoms revealed an inverse relationship between solvation pressure and the distance between the channel wall and the first liquid layer. The phenomenon of interface slip was also investigated in terms of comparison of reported slip behaviors from the literature, compression of the range of slip data through scaling by system size, identification of the location of slip between the channel walls, and development of a relationship between slip to solvation pressure in which slip is considered to be a rate process. Lastly, the behaviors of shear thinning and oscillation of viscosity with film thickness were characterized using molecular simulations run at variable shear rate and channel width. A composite thin film viscosity model was developed incorporating both effects. During the investigations of these four individual thin film properties, relationships between them were identified (e.g. dependence of solvation pressure on density or interface slip on solvation pressure). The consistency of trends in their behavior suggests that they can be quantitatively related – a significant contribution to a field in which very few research groups have the capacity for simulation-based or experimental investigation of more than one thin film behavior.

In addition to the separate continuum and molecular-scale contributions, and perhaps more significantly, an in depth understanding of the two different modeling approaches was developed. This provides the groundwork that is essential for continued progress towards the high level goal, integrated continuum-molecular modeling. The initial phases of integrated modeling were discussed based on the effect that unique thin film behaviors might have on the continuum models that describe lubricated contact. This analysis revealed many potential overlaps that would be critical parts of an integrated model. Such models would enable not only improved understanding of the behavior of thin film lubricated interfaces, but also, ultimately, provide tools for design of efficient thin film lubricated applications. In addition, this approach is part of a growing trend in scientific research in which multi-scale models are not only preferable, but are sometimes necessary, in order to fully capture the behavior of today's decreasingly smaller and more complicated engineering applications.

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## **Publications**

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