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Development of a new mechano-chemical model in boundary lubrication[☆]

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ABSTRACT

A newly developed tribochemical model based on thermodynamics of interfaces and kinetics of tribochemical reactions is implemented in a contact mechanics simulation and the results are validated against experimental results. The model considers both mechanical and thermal activation of tribochemical reactions instead of former thermal activation theories. The model considers tribofilm removal and is able to capture the tribofilm behaviour during the experiment. The aim of this work is to implement tribochemistry into deterministic modelling of boundary lubrication and study the effect of tribofilms in reducing friction or wear. A new contact mechanics model considering normal and tangential forces in boundary lubrication is developed for two real rough steel surfaces. The model is developed for real tribological systems and is flexible to different laboratory experiments. Tribochemistry (e.g. tribofilm formation and removal) and also mechanical properties are considered in this model. The amount of wear is calculated using a modified Archard's wear equation accounting for local tribofilm thickness and its mechanical properties. This model can be used for monitoring the tribofilm growth on rough surfaces and also the real time surface roughness as well as changes in the λ ratio. This model enables the observation of in-situ tribofilm thickness and surface coverage and helps in better understanding the real mechanisms of wear.

1. Introduction

Boundary lubrication is the lubrication regime where the interface behaviour is dominated by chemical reactions that happen at the surfaces, tribofilm formation occurs, and the load is carried by the asperities. In the boundary lubrication regime the asperity-to-asperity contacts (Fig. 1) may lead to elastic or plastic deformation or even fracture and can generate frictional heat which will be accompanied by chemical reactions to produce organic and inorganic surface films. A wide range of studies regarding many aspects of tribofilm formation and removal and their roles in reducing friction and wear have been conducted [1,2].

The effectiveness of boundary lubrication has been considered for a long time as a necessity for modern designs of machines with reliable operations. Because of the need for more energy efficiency, availability of new materials and machine part downsizing, the need for understanding true interactions in this regime is of great importance. The boundary lubrication regime has been the subject of many studies for more than 70 years [3,4] and the majority of these studies are experimental investigations into the nature of what happens in this regime. Many of the studies cover the boundary film chemical [5,6], physical and mechanical properties [7–11] and their effects on wear and friction reduction. The subject of many works has been to investigate different kinds of additives in oils and their effects on various aspects of tribological performance [1,2,12]. As the boundary lubrication regime is mainly related to interactions of two surfaces and the additive containing oils between them, the analytical studies of surfaces including topography measurements, chemical analyses, mechanical and physical studies are considerable. All these experiments give good insight into different chemical and physical characteristics covering various aspects of boundary lubrication systems.

It is clear from the wealth of experimental literature in this area that the nature of the phenomena happening in this regime is very complicated. Studying the entire problem needs a multiscale understanding ranging from component scale down to the micro-scale and also molecular interactions of films and lubricant additives. Experimentation across such scales is challenging and hence it is important to complement such studies with the ability to predict the friction and wear of a working system without running experiments. It is also important to analyse the system and optimise its performance in order to design cost effective experiments. Many modelling attempts have been made in the past years but a comprehensive multiscale model of boundary lubrication considering tribochemistry phenomena in order to predict friction and wear of the system is still lacking.

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Nomenclature

p	normal pressure (Pa)
V^*	complementary potential energy (J)
$\bar{u}_z, u_x, u_y, u_z$	surface deformations (m)
$\bar{u}_z^*$	surfaces prescribed deformation (m)
E_1, E_2, E^*, G^*	elastic and shear modulus (Pa)
q, q_x, q_y	tangential pressure (Pa)
v_1, v_2	Poison ratio
C_{kl}	coefficient matrices
a, b	discretised area length (m)
t	time (s)
$k_{\text{tribo-thermo}}$	tribochemical reaction rate constant (s^{-1})
k_{thermo}	thermal reaction rate constant (s^{-1})
x_{tribo}	tribo-activation reaction factor
x_{thermo}	thermal activation reaction factor
k_1	Boltzmann constant (m^2 kg s^{-2} K^{-1})
T	temperature (K)
h'	Planck's constant (m^2 kg s^{-1})
ΔE	activation energy (J)
R	gas universal constant (J mol k^{-1})
A, B, C	chemical concentrations (mol)
h_{max}	maximum film thickness due to formation
h	tribofilm thickness
C_3, C_4	removal constants
C_1, C_2, A_1	tribofilm formation constants
E_f^*	tribofilm elastic modulus (Pa)
E_{0f}^*	threshold elastic modulus (Pa)
H_0	tribofilm threshold hardness (Pa)
H	tribofilm hardness (Pa)
K	dimensionless Archard wear constant
COW_{tr}	Archard's wear coefficient for tribofilm
COW_{steel}	Archard's wear coefficient for steel
COW_{min}	Archard's wear coefficient for steady state tribofilm

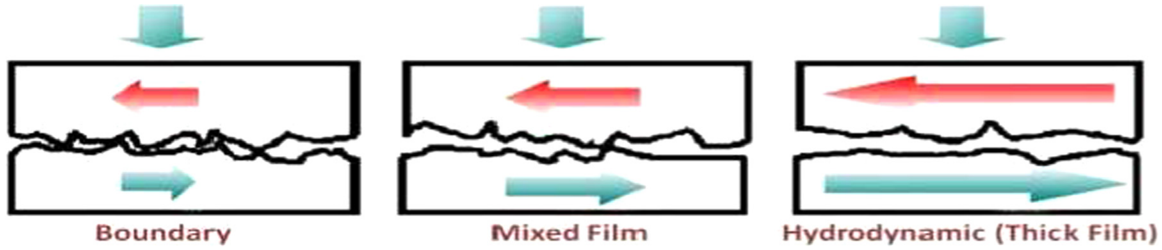

Fig. 1. Lubrication regimes.

Sullivan [13] developed a model for oxidational wear under boundary lubrication. He proposed a mathematical model which relates the wear to applied load and pressure and involves many other factors that together can be assumed as Archard's wear equation coefficient. However, there is no detailed contact mechanics in this model. Stolarski [14] developed a model for wear prediction in boundary lubricated contacts both in dry and lubricated contact between sliding surfaces. He used statistical models and probability functions to predict the asperity–asperity contact, determining the probability of elastic or plastic contact and thus calculating the wear. That approach used the Greenwood and Williamson model of contact mechanics [15]. Zhang et al. [16] derived a model for micro contacts. The deformation of asperities in this model can be elastic, elasto-plastic or even fully plastic and the possibility of contacts are determined by a contact probability equation. They used the Jaeger equation [17] over the contact area in order to calculate the asperity flash temperature. Classical wear theories were used for calculating the probability of contact covered by oxide layer and also probability of contact covered by physically and chemically adsorbed layers were studied.

Recently, Bosman et al. [18] proposed a numerical model for mild wear prediction under boundary lubrication systems. They assumed that the main mechanisms that protect the boundary lubricated system are the chemically reacted layers and when these layers are worn off, the system will restore the balance and the substrate will react with the oil to produce a tribofilm. They also proposed a transition from mild wear to more severe wear by making a complete wear map. Hegadekatte et al. [19] developed a multi-time-scale model for wear prediction. They used commercial codes for determining their contact pressure and deformations and then used Archard's wear equation for calculating wear. Andersson et al. [20] used a wear model and implemented FFT based contact mechanics simulations to calculate contact pressure and deformations.

Another recent work by Andersson et al. [21] used contact mechanics of rough surfaces considering the tribofilm properties and also the tribofilm formation and growth. They used an Arrhenius equation for the tribofilm growth and Archard's wear equation for wear predictions. The novelty of this work was considering the tribofilm and also film formation rate during the time. The film formation was following an exponential formulation based on Arrhenius equation. The model was based on contact pressure and flash temperature and these parameters were responsible for tribofilm growth. They calibrated their tribofilm equation at the local scale and calculated the average tribofilm at the global scale. The model considered the tribofilm thickness and the hardness variation through the film but did not consider the elastic properties of the tribofilm. They used a simple form of Archard's wear equation and calibrated the equation based on experimental results. The work presented here was considered as a modification to that work but there are several improvements in this model that are highlighted in the paper.

Despite the important role tribochemistry plays in the behaviour of tribosystems, there is no comprehensive modelling framework that considers tribochemistry in boundary lubrication. The main aim of this work is therefore to build such a framework to implement tribochemistry into boundary lubrication modelling that can predict friction and wear of the system with respect to the effect of the tribofilm.

The importance of tribofilms and an attempt to find the true mechanisms involved in reducing wear and friction will be studied in this work. The model was built in a way that it would be flexible for various working conditions and different real tribosystems as well as different additives and their concentrations.

2. Components of the model

To study the contact of real rough surfaces, digitized rough surfaces are important inputs of all numerical studies. These digitized surfaces can be either generated mathematically or can be obtained from surface measurement instruments like Atomic Force Microscope.