Tribology International 107 (2017) 33–38

Contents lists available at ScienceDirect

Tribology International

journal homepage: www.elsevier.com/locate/triboint

# Study of the Interfacial Mechanism of ZDDP Tribofilm in Humid Environment and its Effect on Tribochemical Wear; Part II: Numerical

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ARTICLE INFO

*Keywords:*
ZDDP
Boundary lubrication
Relative humidity
Wear

ABSTRACT

Relative humidity and the effect on tribochemistry and wear of boundary lubricated systems are examined experimentally in part one of this study. In part II of this study the tribofilm thickness and wear results obtained experimentally are used to develop a semi-deterministic approach to implement the effect of humidity in wear prediction of boundary lubrication for the first time. Two approaches were used for this purpose; firstly, a modification factor was found to be suitable for Archard's wear equation to be able to account for the effect of relative humidity. This factor is found to be good for engineering designers to be able to predict the lifetime of machine parts. Secondly, the effect of humidity on the tribofilm growth on the surfaces was captured in the model and its effect on wear was tested based on a recent model developed by the authors. It is shown that, as expected, if the tribofilm growth is captured effectively, wear can be predicted. The prediction results were validated with the experimental results showing good agreement. Calibration of the tribochemical model at different levels of relative humidity suggest that the maximum tribofilm formation factor ($h_{max}$) is varying linearly with the humidity percentage. This led to the further development of the tribochemical model of the authors to adapt to the humid environments.

## 1. Introduction

Previous investigations revealed that water which comes from the environment plays a critical role in the damage process of oil-lubricated tribological systems [1–7]. Corrosion or hydrogen embrittlement could occur in the presence of water in oil which plays a significant role in causing accelerated wear [8–14].

### 1.1. Effect of water on lubrication

Additives present in the lubricant can be decomposed by small amounts of water and produce sludge and acid which are harmful for every tribological system [11]. Rounds et al. [15] found that the presence of water in the oil changes the decomposition rate of the ZDDP. Water molecules can also prevent the additive molecules reacting with the substrate to form a protective reaction layer on the contacting surfaces due to the fact that the non-polar head of water molecules points out to the surrounding oil while the hydrophilic polar heads assemble in the centre and surround the polar additive molecules [3,11,12,16].

It was also proposed by Faut et al. [17] that water delays the formation of the tribofilm on the surface which can affect the wear process of the system. The same trend was observed by Parsaeian et al. [12]. Water has a big influence on the additive-containing oils because of the hydrophobicity of these oils [11,18–20]. Another way that water can influence the lubricant properties is to change the solubilisation characteristics of the lubricant which results in the de-solubilisation of the additive in the lubricant [11]. It was shown that contacting surfaces can be affected in humid conditions by mechanochemical reactions involving the adsorbed water which can be attributed to hydrolysis reactions enhanced by interfacial shear [21].

It was reported that thinner tribofilms are formed on the surface at higher levels of relative humidity and higher water concentration which can strongly affect the wear performance [11,12,16,22]. Parsaeian et al. [12,16] found that water can affect the performance of ZDDP by altering the polyphosphates chain length. This effect manifests itself in the formation of shorter polyphosphate chain at higher levels of relative humidity [16,23]. The results are in a good agreement with the study done by Nedelcu et al. [24].

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http://dx.doi.org/10.1016/j.triboint.2016.11.015
Received 12 September 2016; Received in revised form 28 October 2016; Accepted 7 November 2016
Available online 15 November 2016
0301-679X/ 

### *1.2. Wear prediction*

Wear prediction has been the subject of many research papers in the past few decades in order to predict the lifetime of machine elements. Because of the complicated nature of the processes occurring, a universal wear model that is able to fully predict the whole process considering the physical, chemical and mechanical aspects is still lacking. However there are numerous wear models in the literature [25] which can predict wear in specific working conditions or are valid for particular mechanism of wear [26–29].

Archard's wear equation was widely used in the literature to predict wear in lubricated and unlubricated conditions in different contact configurations and also different length scales [30,31]. It is clear that the chemistry of lubricants and the chemical and mechanical interactions at the interfaces are significantly important in the wear of boundary lubricated contacts. Hence it is important to develop models that can capture these important properties of interfaces.

In some recent studies, tribochemistry was considered in modelling of boundary lubrication. Andersson et al. [32] developed a mathematical model using an Arrhenius-type equation for the formation of the tribofilm on contacting asperities and used mechanical properties of the tribofilm to calculate plastic deformations. Bosman et al. [33,34] used diffusion reactions to capture the growth of tribofilm on the surfaces. They proposed a new wear model that considers partial removal of the tribofilm responsible for mild wear of boundary lubricated contacts.

More recently, Ghanbarzadeh et al. [35] used a mechano-chemical approach to develop a tribochemical model for the formation and removal of the tribofilm and modified the Archard's wear equation to account for the effect of the tribofilm. The wear model was validated against experimental wear measurements for different temperatures and showed good agreement [36]. The model suggests that a good prediction of the tribofilm will result in a fairly good prediction of wear in the case of antiwear tribofilm formed on steel substrate. The same model was used in another work of the authors to predict the tribocorrosive wear of boundary lubricated systems in the presence of water [12]. Two numerical approaches were used in the paper to predict tribochemical wear in the presence of water. In the first approach, the Archard wear coefficient was modified with a factor to account for the effect of water. In the second approach, coefficient of wear was assumed to be constant and the effect of tribofilm was considered for all different levels of water content. It was shown that if the growth of the tribofilm can be captured, the wear can be predicted using the model reported in Refs. [35,36].

This study indicates incremental improvement to a recently developed tribochemistry model which is capable of predicting wear and tribofilm growth in humid environment. For this purpose, a set of experimental results reported in another paper of the authors [16] (first part of this study) was employed to calibrate and validate the model. The experimental results reported in Ref. [16] include the tribofilm thickness measurements at different levels of relative humidity as well as wear measurements on the samples. The results are then used to predict wear in two different numerical approaches that will be explained in detail in Section 4. The discussion on the numerical approaches is reported in Section 5.

## 2. Experimental results

To investigate the effect of relative humidity on tribofilm formation and wear of the system, a set of experiments was carried out by using Mini Traction Machine (MTM) with the Spacer Layer Interferometry Method (SLIM) attachment. A humidity control system was designed to monitor relative humidity during the experiments. The experimental results reported in detail in the first part of this study [16].

Figs. 1 and 2 illustrate the effect of different levels of relative humidity on tribofilm thickness. The results show that the higher

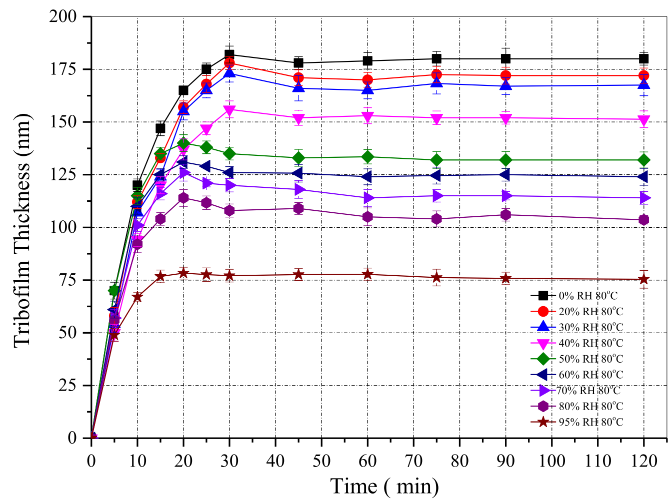


**Fig. 1.** Tribofilm thickness measurement results at 80 °C for different levels of relative humidity.

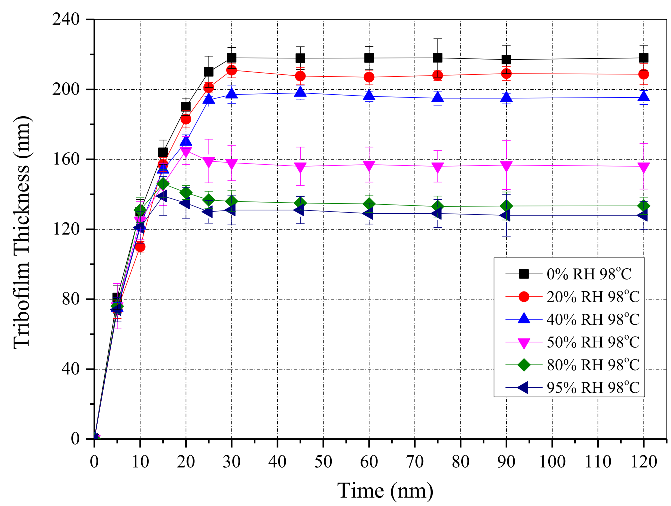


**Fig. 2.** Tribofilm thickness measurement results at 98 °C for different levels of relative humidity.

tribofilm thickness was observed at lower relative humidity for both temperatures while the thickness of the tribofilm reduced by increasing the relative humidity. The lowest tribofilm thickness was found at the highest value of the humidity for both temperatures. Fig. 3 indicates that the average wear depth for both temperatures increased by increasing the humidity but it is more noticeable for lower temperature and higher humidity due to the higher water concentration in the oil.

## 3. Numerical model

The model used in this work is the semi-deterministic approach developed by authors in Refs. [36,37]. The model was modified to account for the effect of water and its tribochemistry on the wear performance of boundary lubricated contacts in the presence of ZDDP as an anti-wear additive [12]. The details of the numerical model and its validations are reported in detail in Refs. [36,37]. However, the components of the model are presented here. The model consists of three important parts:

I. A contact mechanics code for rough surfaces assuming an elastic-perfectly plastic material response;
II. A semi-analytical tribofilm growth model which includes both tribofilm formation and partial removal; and
III. A modified Archard's wear equation which accounts for the local