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Towards optimum additive performance: Understanding the influence of roughness parameters on the ZDDP tribofilm growth by simulation

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ABSTRACT

In recent years, several theoretical models to predict the triboreactive film thickness of zinc dialkyldithiophosphates (ZDDP) have been developed. Although these models are not complete and are approximate in nature, they provide a framework which can be used to evaluate the factors impacting the tribofilm growth. In this paper, rough surfaces with different roughness parameters were numerically generated and used to calculate the tribofilm growth. The simulation results show that lower negative skewness, higher kurtosis, and larger autocorrelation length values give thicker ZDDP tribofilms with skewness and autocorrelation values having a greater effect on the tribofilm growth. Based on the simulation results, it is found that these parameters influence the tribofilm growth by changing the contact ratio which eventually changes the dynamic growth of tribofilm and wear of substrate. The results presented in this paper have bigger implications for industry in designing surface textures that promote the anti-wear action.

KEYWORDS: Roughness parameters; ZDDP; Tribofilm growth; Modeling

1. Introduction

Zinc dialkyldithiophosphates (ZDDP) is the most widely used anti-wear lubricant additive[1]. The key reason for the remarkable anti-wear performance of ZDDP is the thin film formed by chemical reaction in the contact interface, named as tribofilm. In recent years, with the use of advanced in-situ experimental techniques, sliding friction between two contact surfaces has been confirmed as the dominant factor that initiates and sustains chemical reactions between interacting surfaces. The complete process of tribofilm growth is considered as a combination of tribofilm formation, removal, and replenishment[1]. The ZDDP tribofilm provides protection under extreme conditions of boundary and mixed lubrication. The additive is always present in the lubricant and only comes into action under extreme conditions of high shear or asperity contact, forming thick sacrificial layers that ultimately reduce wear. The formation and removal mechanisms of these layers and their chemical nature have long been an active area of research. The more recent studies are focusing on understanding the transient formation of these films[2-6] using in situ tools and devices.

The nature of these tribofilms has been the subject of study for decades and much is known about the antiwear action of ZDDP. It reduces wear by forming tenacious films on top of asperities between contacting bodies[7]. These films contain amorphous phosphate glasses[8,9] which can be formed by thermal energy alone (thermal films) or thermal and mechanical energy together (tribofilms). Both thermal and tribofilms have similar composition and have been shown to form on several substrate materials including ferrous[10] and non-ferrous[11-14] materials and can reach a mean thickness of around 200 nm[15]. It should be noted that the thermal films on ferrous contain less iron than the tribofilms and the main cation is zinc[16].

The understanding of tribofilm kinetics makes it possible to develop models of tribofilm growth and this eventually helps both academia and industry to learn the growth process and understand the evolution of properties of the tribofilm and hence, optimize the performance of tribopairs. Several mechanisms have been proposed for the formation of tribofilms[17] like flash temperature rise[18], pressure based cross-linking[19], triboemission[20], surface catalysis etc. but the stress-promoted thermal activation process is considered to be the most well accepted idea[17,21] and explains the formation of tribofilms at much lower temperature compared to the thermal films that form only at much elevated temperatures. This states that the presence of shear stress reduces the required effective activation energy for the forward reaction. Therefore, the growth of tribofilm can be related to all or a subset of these phenomenon when developing a model for tribofilm growth.

Based upon the discussion provided above, it is obvious that achieving a true tribofilm growth model is a complex and difficult task. Therefore, most of the tribofilm growth models that have been developed until now, make use of approximated constants that are derived from experiments or are based on experience. The current approaches to include a tribofilm growth modelling into contact mechanics simulations relies on establishing a framework that includes: a contact mechanics / lubrication model, a tribofilm growth and removal model, a tribofilm mechanics model, and a wear model[22-27]. All these respective components are interlinked and the information travels between these sub-models to simulate realistic tribofilm growth experiments.

The surface roughness can improve the friction and wear performance by enabling accumulation of lubricant within the micro-features to provide a secondary supply of lubricant[28,29], trapping abrasive worn particles to reduce abrasive wear[30-32], and improving the hydrodynamic pressure buildup to enhance lubrication[33,34]. Roughness has also been found to affect the transition of lubrication regimes and in some cases the micro-features on the rough surfaces postpone the transition to boundary lubrication[35]. Tomanik et al.[36] suggested that the hydrodynamic load support increased by almost 50–90% when laser surface texturing was employed. Most studies focus on understanding the effect of micro-texture (micro-feature) geometry (size and shape etc. of features) on the tribological performance of interfaces[37-43].

Recently, studies have started linking the statistical roughness parameters to the tribological performance of surfaces textured with simplified geometries like dimples[44,45]. They employed contacting pairs between steel-tin, steel-aluminium and steel-polymers, and found that the friction performance and transfer layer formation were independent of the simple roughness parameters like arithmetic mean of roughness. Instead other texturing parameters like the average slope of the surface roughness profile were found to be the key factors influencing friction and wear[46].

The presence and buildup of tribofilm during sliding can have significant effect on the tribological performance of textured surfaces[47]. Until now the understanding of the effect of roughness on the growth of tribofilms is missing and no framework or instructions are available that link the performance of surfaces to grow tribofilm to the roughness parameters. Brizmer et al.[24] performed simulations to study the effect of R.M.S. roughness on the mean tribofilm growth but only three data points were used to develop a curve. Nevertheless, they showed that the mean tribofilm thickness increases as the R.M.S roughness increases. Some studies have indirectly given evidence about the effect of roughness on tribofilm growth or vice versa. Recently, a study[48,49] suggested that surface textures that result in greater pressures, thicker lubricant films and greater contact area hold promise for optimal performance under tribochemically active conditions. Azam et al.[27] performed a simulation study and suggested that the growth of tribofilm leads to increased lubricant entrapment. This was thought to be due to retention of deeper grooves in the roughness geometry which are representative of non-Gaussian surfaces. Another study performed by Xu et al.[50] recently accessed the effect of dimple shape on the formation of tribofilms and suggested that under starved conditions, the tribological performance of these surfaces (to generate and sustain tribofilms) was influenced by the geometry of the dimples and there is an optimum value of major to minor axis ratio for achieving optimal performance.

However, the previous studies were either focused on the development and calibration of the tribofilm growth models or were mainly accessing the performance of certain surface texturing parameters. Even when linking tribofilm growth to the roughness parameters, only the root-mean-square (R.M.S.) roughness (S_q) is considered. The latest ISO 25178-2:2012[51] suggest that a series of key parameters is needed to comprehensively characterize the surface topography. Moreover, different manufacturing processes generate a variety of rough surfaces with different features.

Thus, only using root-mean-square roughness is not adequate to characterize the rough surfaces.

Therefore, the current study set out to highlight the key roughness parameters affecting the growth of ZDDP tribofilms. Rough surfaces with more comprehensive characteristic parameters were generated numerically[52] and then selected roughness parameters were calculated based on the ISO 25178-2:2012[51]. These rough surfaces were given as input to the tribofilm growth modelling framework. It is necessary to point out that these input rough surfaces will experience running-in period even before the formation of tribofilm. However, the formation of ZDDP tribofilm during sliding contact is believed to be fast[1]. Therefore, it is rational to ignore the running-in period before the formation of the tribofilm without losing the true representation of the input surfaces. The model of Ghanbarzadeh et al.[23] was used in present work to simulate tribofilm growth due to its flexibility and ease of use. The tribofilm growth model has been validated against several experimental scenarios and has been found to give very good match against experiments [1, 2, 3, 4, 5, 6] and this make the arguments presented in this study physically valid.

The growth trend and equilibrium thickness of tribofilm were compared between surfaces with different roughness parameters. The roughness parameters that are the most relevant to the tribofilm growth were emphasized and recommendations are made to use these parameters to develop optimal rough surfaces for targeted performance in a tribochemically active system. For systems where only limited amounts of ZDDP are used in order to limit phosphate ash, phosphorus and sulfur in the exhaust[53,54], the study will provide a good way to enhance the tribofilm growth performance to maintain the antiwear performance.

The paper first, briefly introduces the selected roughness parameters and brief details of the tribofilm growth model used. This is then followed by the results and discussion section where the effects of the roughness parameters on tribofilm thickness are presented. The key roughness parameters are identified before concluding the study with some recommendations on optimizing the antiwear tribofilm thickness by controlling the surface roughness.

2. Selected roughness parameters

In order to initialize the parametric study, rough surfaces with different parameters are required. Generally numerical methods are used to generate rough surfaces because it gives the ability to generate surfaces with various features, conveniently. This gives roughness as a matrix of random numbers with specific distributions. Several roughness parameters[51] are used to define this distribution of roughness e.g. the root-mean-square roughness (S_q), skewness (S_{sk}), kurtosis (S_{ku}), and autocorrelation length (S_{al}) etc. In current work, the method previously proposed by the authors is used to generate rough surfaces[52].

The roughness parameters mentioned above only describe the overall features of rough surfaces which may not provide adequate information to comprehensively understand the influence of rough surfaces on the tribofilm growth. This is crucial as the chemical reaction is believed to be occurring at the asperity contact spots. Therefore, some parameters specifically related to the asperity scale[55] should be included in the parameter set and these are: the mean summit curvature, S_{sc} and density of asperities (summits), S_{ds} .

To further explain the meaning of each of the selected parameters, the mathematical definitions are presented below:

Root-mean-square roughness (S_q)

$$S_q = \sigma = \sqrt{\frac{1}{A}\iint_A z^2\left(x, y\right)dxdy} \tag{1}$$

Skewness (S_{sk})

$$S_{sk} = \frac{1}{\sigma^3}\left[\frac{1}{A}\iint_A z^3\left(x, y\right)dxdy\right] \tag{2}$$

Kurtosis (S_{ku})

$$S_{ku} = \frac{1}{\sigma^4}\left[\frac{1}{A}\iint_A z^4\left(x, y\right)dxdy\right] \tag{3}$$

Autocorrelation length (S_{al})

$$S_{al} = \min_{t_x, t_y \in R} \sqrt{t_x^2 + t_y^2} \text{ , where } R=\left\{\left(t_x, t_y\right) : f_{ACF}\left(t_x, t_y\right) \le s\right\} \tag{4}$$

The mean summit curvature (S_{sc})

$$S_{sc} = \frac{-1}{2n}\sum_{i=1}^{n}\left(\frac{\partial^2 z\left(x, y\right)}{\partial x^2}\right) + \left(\frac{\partial^2 z\left(x, y\right)}{\partial y^2}\right) \tag{5}$$

The density of summits (S_{ds})

$$S_{ds} = \frac{n}{A} \tag{6}$$

where z is the surface height distribution of the evaluation area, A is the evaluation area, n is the number of summits of the surface, a summit is defined as the point which is higher than all the adjacent points, s is the truncation coefficient defined in the calculation of autocorrelation length. Its recommended value is 0.2 in ISO 25178-3:2012[56]. S_{al} is defined on the basis of the autocorrelation function, f_{ACF}, shown below

$$f_{ACF}\left(t_x,t_y\right)=\frac{\iint_A z\left(x,y\right)z\left(x-t_x,y-t_y\right)dxdy}{\iint_A z\left(x,y\right)z\left(x,y\right)dxdy} \tag{7}$$

In this paragraph, the physical meaning of each of these parameters is quickly explained. The parameters S_q, S_{sk}, and S_{ku} determine the height distribution of rough surfaces. The parameter S_{al} defines the horizontal distance of the f_{ACF} which has the fastest decay to the specified value s (0.2). The two, asperity scale parameters, the density of summits, S_{ds} and the mean summit curvature, S_{sc} are defined as the ratio of number of local maximum points in the evaluation area and the mean curvature value of all local maximum points, respectively.

3. ZDDP tribofilm growth model

It is important to mention that the focus of present study is on the influence of roughness parameters on the growth of tribofilm. The study uses an already developed model and applies it on various rough surfaces with predefined features and characteristics to understand the relative importance of each of these parameters in forming tribofilms. Therefore, in this section the tribofilm growth model is explained briefly.

The detailed information of the model can be found in the work of Ghanbarzadeh et al.[23] whereas the schematic flow chart of the framework specific to the current study is given in Figure 1. In summary, the tribofilm growth modelling framework contains four sub-models which are, the *contact mechanics model* for simulating the contact of rough surfaces, the *tribofilm formation and removal model*, model to consider the *modifications of tribofilm mechanical properties* on the overall contact performance, and the *wear model considering the effect of tribofilm* growth.

In the following each of these sub-models is explained in the context of the overall tribofilm growth framework. As the first step, the rough surface data for both the counter bodies is given as input to the contact mechanics model. In the current study, the contact mechanics model proposed by Almqvist et al.[57] is used to find the contact status and pressure distribution between the two contacting rough surfaces. This model considers both the elastic and plastic deformation of rough surfaces. The next step involves the use of an empirical formula (Equation 8), describing the formation and removal of tribofilm at local contact points to estimate the tribofilm thickness distribution at a given time step. At this stage, the tribofilm thickness is a localized distribution of numbers defining the asperity scale height of the tribofilm. It is well known that the tribofilm has different mechanical properties compared to the substrate. Therefore, in the next step, the effect of generated tribofilm on the mechanical properties of surfaces is considered in an approximate way as given by Andersson et al.[22] and Ghanbarzadeh et al.[23]. The growth of tribofilm affects the localized wear of the substrate and this is taken into account by assuming the wear to vary among points of different tribofilm thickness. The procedure adopted is the same as given by Ghanbarzadeh et al.[23]. This ensures that the antiwear action of tribofilm is considered by modifying the Archard wear model. The final step involves an update of roughness data. Before the start of the new time step, the roughness distribution is first updated with the asperity scale wear, plastic deformation and tribofilm growth values and then the roughness distribution matrix is circulated to consider the movement of the contacting surfaces. This process is repeated until a predefined time value is reached.

The growth of the tribofilm is considered using Equation 8 as,

$$h = h_{\max}\left(1-\exp\left(-\frac{k_1 T}{h^{'}}\cdot x_{tribo}\cdot t\right)\right)-C_3\left(1-\exp\left(-C_4 t\right)\right) \tag{8}$$

where k_1 and h' are the Boltzmann and Plank's constant, T is the local temperature considering flash and bulk temperature in the unit of Kelvin, and t is the time from the beginning of the rubbing process. There are two calibration parameters, h_{max} and x_{tribo}, and these are obtained from experimental fitting. The parameter h_{max} represents the limiting value of the thickness of the tribofilm and the parameter x_{tribo} is the factor which represents the role of mechanoactivation in initiating the reactions that result in generation of tribofilm. The flash temperature used in this work is calculated based on Jaeger's moving heat source analysis according to Ghanbarzadeh et al.[23]. The parameters C_3 and C_4 are removal constants and are also calibrated based on experimental results. For the current study, all calibrated parameters are taken from reference[23]. This is because the focus of the current study is the relative growth of tribofilm in surfaces with different roughness parameters. Therefore, the effect of different tribofilm growth models or the role of different calibration parameters does not affect the understanding gained in this study.

The roughness data is generally available as computer generated roughness or real scanned roughness information. The rough surface data is input to the contact mechanics model to calculate the contact status and the properties of the interface, which is then used as input to the tribofilm growth and removal model to calculate the localized tribofilm thickness. This not only changes the localized surface heights but also results in localized changes in the mechanical properties of contacting materials as the tribofilm has different properties compared to the substrate. This ultimately affects wear of the substrate material. Finally, the surface topography is updated with the relevant tribofilm growth, tribofilm removal and wear of the substrate, and the contact mechanics model is run again with this updated information. This procedure repeats until the tribofilm thickness distribution has reached dynamic equilibrium. The key concern in these models is that the tribofilm growth is predicted using empirical formulae calibrated through experiments, and the position and amount of generated tribofilm are determined by the contact status of the interface, which is directly influenced by the surface topography. This makes the whole process semi-empirical.

4. Results and discussion

In this section the tribofilm growth from all the rough surfaces is presented. First, the numerical delicacies in the generation of rough surfaces are presented to create benchmark for rough surfaces and to ensure that the generated rough surface data is reliable. Then the tribofilm growth results are presented as a function of the different roughness parameters. At the end of this section, discussion around the possible mechanisms of tribofilm growth enhancement are presented and the implications of this study are outlined.

4.1 Surface generation results

As mentioned earlier, most studies focus on the root-mean-square roughness, S_q, as being the key influencing factor but in the current work skewness, S_{sk} kurtosis, S_{ku} and autocorrelation lengths, S_{al} were also taken as independent variables when generating rough surfaces. These parameters collectively give the statistical or overall behavior of a rough surface. To understand and relate the tribofilm growth to asperity scale, the mean summit curvature, S_{sc} and the density of asperities (summits), S_{ds} were calculated for each of the generated rough surfaces, to provide further insight into the role of roughness in controlling tribofilm growth and to understand the underlying mechanisms.

First of all, Gaussian surfaces (S_{sk} = 0, S_{ku} = 3) with various autocorrelation length values (1, 3, 5, 7, 9 and 11) were simulated to investigate the influence of autocorrelation length on tribofilm growth. The resulting rough surfaces were indexed from 1 to 6, respectively. The rough surfaces used to study the influence of skewness and kurtosis were simulated based on a fixed value of autocorrelation length. This fixed value was taken as 3 in both x and y directions. Then, surfaces with different kurtosis values (S_{ku} = 4, 7, 10, 20) were generated while keeping the skewness value fixed at -0.5. Thus, enabling the study of the influence of kurtosis on tribofilm growth. Finally, to study the influence of skewness on the tribofilm growth, surfaces with different skewness values (S_{sk} = -2, -1, -0.5, 0.5, 1) were generated while keeping the kurtosis value fixed at 7.

On a numerical grid, each rough surface has 128×128 points. The sampling space for each of these surfaces is determined by the solution domain of the contact mechanics model. In this study, the solution a square solution domain is chosen with side length equal to six times the radius of Hertzian contact zone.

The asperity scale parameters S_{sc} and S_{ds} were calculated for each of these surfaces and are given in Table1, 2 and 3. Figure 2 and Figure 3 give the three dimensional views of the generated surfaces to illustrate the influence of the S_{sk} and S_{ku} values on the rough surfaces and the influence of different autocorrelation length values, respectively. It can be seen that larger autocorrelation length values provide larger and smoother asperities.

4.2 Tribofilm simulation results and discussion

In order to conduct a tribofilm kinetic growth simulation, a set of initial parameters are provided in Table 4 and these parameters were kept fixed for simulating the tribofilm growth for all the rough surfaces. Each rough surface is taken as the starting point for each of the tribofilm growth simulation cases presented.

It is important to mention that the tribofilm thickness calculated is much lower compared to the experimentally measured tribofilm thickness value. The reason for such differences is the different ways of computing the average tribofilm thickness in the simulations and experiments. The tribofilm thickness values reported in this study were obtained by averaging the tribofilm thickness in the entire Hertzian contact zone at any given time step. Unlike simulations, the reported experimental tribofilm growth values are obtained by measuring tribofilm thickness in zones selected manually within the Hertzian contact region and the usual practice is to report the tribofilm thickness values for the significant tribofilm pads while neglecting the regions with low or zero tribofilm thickness values. Therefore, the calculated value in this study is much smaller than most experimental results. The advantage of averaging the tribofilm thickness over the entire Hertzian contact zone is that it can provide a solid basis to compare the effect of different roughness parameters. Therefore, the findings from the study remain valid.

The steady state tribofilm thickness value represents the average tribofilm thickness value when the dynamic equilibrium is reached between growth of the tribofilm, removal of the tribofilm and the wear of the substrate whereas the maximum tribofilm thickness value represents the highest value of the averaged tribofilm thickness that was achieved during the entire growth process of the tribofilm.

Effect of skewness and kurtosis

In essence, skewness and kurtosis represent the deviation of the roughness distribution from the Gaussian distribution. Figure 4 shows the evolution of tribofilm thickness with time when rough surfaces having different S_{sk} values were used in the simulation. The maximum and steady state tribofilm thickness values are plotted in Figure 5. These results clearly show that with different S_{sk} values, the qualitative trend of tribofilm thickness evolution (with time) is similar but quantitative differences exist. Although the differences seem small but due to the fact that the tribofilm thickness values presented are the mean values for the complete simulation, these differences are significant.

The S_{sk} value also has significant influence on the thickness of the tribofilm. The results suggest that with lower negative S_{sk} values, the tribofilm becomes thicker. For comparison purposes, the tribofilm growth curve with a Gaussian rough surface is also plotted in Figure 4 as a reference. It is evident that, the presence of skewness always results in thicker tribofilms compared to purely Gaussian rough surfaces, irrespective of the S_{sk} values being positive or negative. This behavior suggests that the non-Gaussian surfaces could be beneficial for the growth of tribofilm and improving the antiwear performance of additives.

The tribofilm thickness values with varying kurtosis values are presented in Figure 6 and Figure 7. Figure 6 presents the evolution of tribofilm thickness with time while in Figure 7, the maximum tribofilm thickness and the steady state tribofilm thickness values are plotted. In Figure 6, the tribofilm growth for the Gaussian rough surface is also presented for comparison. The results show that the S_{ku} values also influence the tribofilm growth, with larger S_{ku} values giving thicker tribofilms but the effect of S_{ku} is quantitatively smaller than that of the S_{sk}. However, when different S_{ku} values were considered in the simulation, the resulting tribofilms were always thicker compared to that of the Gaussian rough surface (Figure 6).

Effect of autocorrelation lengths

The tribofilm growth curves for different autocorrelation length values are shown in Figure 8. It can be seen that the autocorrelation length values have a dramatic influence on the tribofilm growth results. The qualitative trend for tribofilm growth remains same but quantitatively, the tribofilm thickness values are quite different. Figure 9 extracts the maximum and steady state tribofilm thickness as a function of different autocorrelation length values. The results suggest that with larger autocorrelation length values, thicker tribofilms grow.

In summary, comparing the trends of tribofilm growth by changing skewness, kurtosis, and autocorrelation length values, it can be said that the skewness and autocorrelation length values have greater effect on the growth of tribofilm than kurtosis values. This result can provide useful instructions for the design of rough surfaces to systematically enhance (control) the tribofilm growth by taking advantages from the manufacturing processes involved in the development of the designed product. For example, it should be a reasonable way to manufacture the counter parts with lower negative skewness and larger autocorrelation length values as this will increase the ability of ZDDP tribofilm to grow thicker films.

Mechanism of roughness parameters influencing tribofilm growth

For all the different rough surfaces generated in this study, the curves of the tribofilm growth exhibit the same trend. Several reasons are possible. First of all, the tribofilm growth model and the corresponding calibrated parameters used are the same for all the rough surfaces. Secondly, the curves presented only differ in the initial starting roughness used to generate each of these curves and it is believed that roughness may cause the tribofilm thickness to change but the growth and removal behavior of the tribofilm will eventually determine the overall trend of the tribofilm growth curves.

In this tribofilm growth framework, the contact mechanics model is the foundation. As discussed earlier, there can be several mechanisms of tribofilm growth and among these the shear activated tribofilm growth is considered as the most important. Under different conditions of contact, different mechanisms of tribofilm formation may be active[17]. The contact conditions in the current study are close to boundary lubrication and therefore, the shear stress is maximum at the contacting asperities. Therefore, the formation of tribofilm is considered to be occurring at the contacting asperities.

According to the above understanding, it is helpful to link the stochastic parameters discussed above with the characteristic parameters of asperities to illustrate the mechanism of enhancement of ZDDP tribofilm growth. In this study, two characteristic parameters of asperities, the mean summit curvature, S_{sc} and the density of asperities (summits), S_{ds}, were selected for this purpose. In addition, the contact ratio (ratio of the area formed by contacted asperities to the area of the Hertzian contact zone) of the rough surfaces is also considered to be one of the key parameters connecting the contact mechanics and tribofilm growth models as it dictates the severity of contact and is linked to the formation of thicker tribofilms.

The parameter S_{sk} describes the asymmetry of the rough surface height distribution. If the value of S_{sk} is equal to 0, a rough surface with symmetric surface roughness height distribution is formed. If the value of S_{sk} is less than 0, it indicates a rough surface with holes whereas if the value of S_{sk} is greater than 0, it describes a flat surface with peaks. It is expected that a bearing surface with holes could provide a larger solid contact area for the growth of the tribofilm. To explore this further, the asperity scale parameters S_{sc} and S_{ds} are given in Table 1 corresponding to the different values of S_{sk}. It can be seen that with increasing S_{sk} values, the S_{sc} parameter decreases while the S_{ds} parameter does not change much. The values of parameter S_{sc} in table 1 indicate that the scale (size) of asperities is larger with larger (positive) skewness, indicating larger contact ratio and hence, the ability to form thicker tribofilms. This is contradictory to what the parameter S_{sk} suggests. In order to clarify these two contradicting opinions, the initial contact ratio values of rough surface with different S_{sk} values were plotted in Figure 10. It shows that with the increase of the S_{sk} value, the initial contact ratio value decreases overall. Note that the initial contact ratio value when S_{sk} equals -0.5 is slightly larger than that when S_{sk} equals -1. This might be due to the numerical errors associated with the process of generation of rough surfaces. But the overall trend of contact area ratio with S_{sk} values has a decreasing trend. Figure 10 also explains why the lower negative S_{sk} values could result in thicker tribofilm, and the higher positive S_{sk} values could lead to thinner tirbofilms. Therefore, the characteristic parameters of asperities cannot be used alone to accesses the capability of rough surfaces as this does not directly relate to the contact of asperities. The S_{sc} value is an average value of all the asperities of the rough surfaces, it does not represent the actual asperities which take part in the contact. when the height distribution of the rough surfaces is not symmetric.

The parameter S_{ku} describes the sharpness of the distribution of heights in a rough surface. A larger S_{ku} value means a sharper height distribution i.e. more height values are distributed near the mean value. In other words, this means that the extreme height values (high or low) are reduced. Without these extreme values, the resulting rough surfaces are flatter, which will ultimately exhibit larger contact ratios and thicker tribofilms. The S_{sc} and S_{ds} values in Table 2 also support this point. When S_{ku} equals to 4 (the smallest in this study), both the S_{sc} and the S_{ds} values are also smallest. This means that although the asperities forming the rough surfaces are large and the number of asperities is small. With increasing value of S_{ku}, the S_{sc} and S_{ds} parameters also increase. Therefore, there are two competing factors linked to the contact ratio. The larger asperities suggest greater contact ratio while being smaller in number suggests smaller contact ratio values. The contact area ratio is plotted as a function of S_{ku} parameter, in Figure 11. It clearly indicates that the greater the S_{ku} value, the greater the initial contact ratio values. It can be readily seen that the changes in contact area ratio with changes in S_{ku} values is not as large as that with changing S_{sk} values (see Figure 10). Such weak influence of S_{ku} on the asperity contacts is expected as changing it will only have a very small influence on the height distribution of rough surfaces. Considering the definition of S_{ku} given in Equation 3, it is linked to the fourth order moment of rough surface height distribution, whose order is higher than S_{sk} (third order moment) and higher order means weaker influence on the height distribution.

The values of the asperity scale parameters S_{sc} and S_{ds} for the different values of autocorrelation length are provided in Table 3. These values suggest that with larger autocorrelation length values, the asperities become larger and smoother. As the autocorrelation length increases, S_{sc} decreases dramatically while S_{ds} decrease slightly. A smaller value of mean summit curvature, S_{sc} indicates larger and smoother asperities and result in large contact ratios and thicker tribofilm growth. To illustrate this further, the initial contact ratio values of all the six surfaces are plotted in Figure 12. It clearly shows that surfaces with larger autocorrelation length values have larger initial contact ratio values. A close look at the values of S_{sc} and S_{ds} in Table 3 and the plot in Figure 12 suggests that the mean summit curvature decreases as the autocorrelation length values increase. On the other hand, the parameter S_{ds} decreases overall to indicate smaller number of asperities as the size of asperities increases. It can be also noticed that the changes in contact area ratio with changes in autocorrelation length values is larger than that with changing S_{ku} values (see Figure 10). As discussed above, S_{ku} has weak influence on the height distribution. On the other hand, autocorrelation length is not defined based on the height distribution, but directly affects the lateral size of asperities. Thus, autocorrelation length should have larger influence than S_{ku}.

In light of the results and discussion provided, the understanding given by the asperity scale parameters and the autocorrelation function in terms of tribofilm growth enhancement support each other but for the non-Gaussian surfaces ($S_{sk} \neq 0$ and $S_{ku} \neq 3$), the understanding gained by the asperity scale parameters alone is not sufficient to explain the tribofilm growth enhancement behavior. And the most reliable parameter to explain such behavior is the contact area ratio.

In summary, the underlying mechanism by which the roughness parameters like skewness, kurtosis, and autocorrelation length affect the tribofilm growth is that by changing the asperity geometry which ultimately changes the contact ratio in the Hertzian contact zone. Higher contact ratio represents thicker tribofilms. It should be noted that although the current study is performed on the ZDDP tribofilm, but the mechanism revealed can be generally applied to all additives which require sliding contact, especially asperity contact, to promote chemical reaction and form thin films.

The surface roughness can be used as an effective parameter in product design to control the tribological performance without changing the original system and operating parameters. Therefore, offering a cheaper and simpler alternative to improve system performance (friction and wear) by avoiding component redesign and being easy to implement in existing and future technologies[58]. This works most efficient when no or very low costs is associated with the development of the required roughness as the benefits obtained might need to be justified over costs[59]. In the current study, it means that the growth of ZDDP tribofilm can be enhanced by optimizing the manufacturing processes to obtain lower negative skewness, higher kurtosis and larger autocorrelation values.

5. Conclusions

In this study, rough surfaces with various skewness, kurtosis, and autocorrelation length values were numerically generated. These surfaces were used as input in a deterministic ZDDP tribofilm growth (kinetic) model. The influence of these roughness parameters on the tribofilm growth was studied. The main conclusions are below:

1 Lower negative skewness, higher kurtosis, and larger autocorrelation length values give thicker ZDDP tribofilms in the simulation with skewness and autocorrelation length values have a greater effect on the tribofilm growth.

2. Skewness, kurtosis, and autocorrelation length values influence the tribofilm growth by changing the contact ratio in the Hertzian contact zone.

3. These results from the current study suggest that the performance of rough surfaces can be tuned to optimize the tribofilm growth. In cases where thicker tribofilms are required, the manufacturing processes can be selected to give counter parts with lower negative skewness and larger autocorrelation length values.

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Nomenclature

A	evaluation area
C_3, C_4	removal constants
f_{ACF}	autocorrelation function
h	tribofilm thickness
h_{max}	limiting value of the tribofilm formation
h'	Plank's constant
k_1	Boltzmann's constant
n	the number of summits of the surface
s	truncation coefficient
S_q	root-mean-square roughness
S_{sk}	skewness value
S_{ku}	kurtosis value
S_{al}	autocorrelation lengths
S_{sc}	mean summit curvature
S_{ds}	density of summits
t	the time from the beginning of the rubbing
T	local temperature
x_{tribo}	factor which represents the role of mechanoactivation in initiating the reactions generating tribofilm
z	rough surface height+

FIGURE CAPTIONS

Figure 1 Schematic flow chart of the simulation model

Figure 2 Examples of the 3D view of the simulated non-Gaussian rough surfaces. a) S_{sk} = -2, S_{ku} = 7; b) S_{sk} = 1, S_{ku} = 7; c) S_{sk} = -0.5, S_{ku} = 20.

Figure 3 Examples of the 3D view of the simulated rough surfaces. a) Surface No. 1; b) Surface No.4; c) Surface No. 7.

Figure 4 Tribofilm growth results with various S_{sk} values.

Figure 5 Maximum and stable tribofilm thickness with various S_{sk} values.

Figure 6 Tribofilm growth results with various S_{ku} values.

Figure 7 Maximum and stable tribofilm thickness with various S_{ku} values.

Figure 8 Tribofilm growth results with various autocorrelation length values.

Figure 9 Maximum and stable tribofilm thickness with various autocorrelation length values.

Figure 10 Initial contact ratio values of rough surfaces with various S_{sk} values.

Figure 11 Initial contact ratio values of rough surfaces with various S_{ku} values.

Figure 12 Initial contact ratio values of rough surfaces with various autocorrelation length values.

TABLE CAPTIONS

Table.1 S_{sc} and S_{ds} values of surfaces with different S_{sk}.

Table.2 S_{sc} and S_{ds} values of surfaces with different S_{ku}.

Table.3 S_{sc} and S_{ds} values of surfaces with different S_{al}.

Table.4 Condition parameters of the simulation.

Table.1

S_{sk}	-2	-1	-0.5	0.5	1
S_{sc} (×10^{-6} 1/nm)	2.12	1.94	1.83	1.57	1.45
S_{ds} (×10^{-3} 1/μm^2)	4.5	4.7	4.8	4.8	4.7

Table.2

S_{ku}	4	7	10	20
S_{sc} (×10^{-6} 1/nm)	1.07	1.83	1.80	1.74
S_{ds} (×10^{-3} 1/μm^2)	3.7	4.8	4.8	4.6

Table.3

S_{al}	1	3	5	7	9	11
S_{sc} ($\times 10^{-6}$ 1/nm)	6.09	4.55	3.70	3.21	2.83	2.62
S_{ds} ($\times 10^{-3}$ 1/μm^2)	1.5	1.2	1.1	1.0	0.98	0.99

Table.4

Parameter	Value
Ball radius R_x / m	0.01
Load p_h / GPa	1.26
Equivalent Young's module E_e / GPa	230
Temperature T_0 / °C	90
Entrainment speed u_s / m/s	0.25m/s
Slide to roll ratio *SRR*	-0.02
RMS roughness of the ball R_{q1} / µm	0.012
RMS roughness of the disc R_{q1} / µm	0.130