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A FEM-Based Study on the Influence of Skewness and Kurtosis Surface Texture Parameters in Human Dental Occlusal Contact

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Abstract

Tooth wear, which manifests with a great variety of degree or level, is one of the dental abnormalities commonly found in diverse populations. The computational modelling of occlusal contact problem can help comprehension of any interaction between teeth generating stress concentration. The approach used to simulate contact between rough surfaces, given the probability density functions, consists in discretizing them into several intervals, so that each one represents a main asperity. The deformations of the main asperities are analyzed and, using homogenization techniques, it is possible to establish the relationship among the responses occurred in micro-scale and the predicted responses in macro-scale. In this work we create parameterized scripts in Python language for the Abaqus CAE software in order to analyze the influence of the surface topography on contact of human dental occlusal surfaces. The texture parameters influence their tribological behavior. As the mean roughness or mean curvature increases, the nature of the contact changes from elastic to plastic and the friction coefficient increases and becomes saturated. For negative skewness, the higher the skewness, the lower the contact area. For positive skewness, the opposite is observed. The higher the kurtosis, greater the area, except for kurtosis less than 3. The surface hardness is not affected by any of the surface texture parameters tested. Further verification using experimental data can encourage dentists to become more familiar with computer simulation.

Keywords:

finite element analysis, contact problem, dental occlusion, surface roughness, height distribution

1. Introduction

Even in the face of increasing prevention of systemic and oral diseases, tooth wear, which manifests with a great variety of degree or level, is one of the dental abnormalities commonly found in diverse populations [1]. This phenomenon occurs physiologically throughout life, slowly and gradually, representing the adaptation of the masticatory system to everyday functions. However this process can change to a pathological pattern. Large tissue loss (enamel and dentin), dentinal hypersensitivity, pulp exposure, loss of vertical dimension of occlusion, poor chewing, change in the contact between teeth and fatigue of masticatory muscles may be consequences of excessive tooth wear [2, 3].

The application of computational techniques in dental research is relatively new and any development that increase the conscious in this area will have an important role in the future. The computational modelling of occlusal contact problem can help comprehension of any interaction between teeth generating stress concentration.

Contact between solid pairs is influenced by a variety of factors including the nature of the materials in contact, the environment in which the chemical interaction takes place, the physical state of the surfaces, the normal force, the relative velocity and the topography of surfaces [4, 5]. When the functionality relative to friction, wear and fatigue is requested, the characterization of surface topography is such a critical factor as the mechanical properties of the involved materials.

There are numerous methods to evaluate the surface texture of a surface [6]. Profilometry, which consists of sliding a thin tip on the surface and conversion of the obtained displacements in a graph, is a major technique to map geometrical parameters and in dentistry it has been used in an attempt to detect earlier surface changes caused by parafunction [7, 8]. Although in vivo measurements is not yet possible to perform, the method is still considered the gold standard [9].

Numerical simulations are useful to evaluate the influence of various operating parameters and to study the phenomenon of friction in a specially

controlled way, computing the strength, the deformation energy and the temperature generated in the process. However, determining the friction is quite complicated, and to overcome this difficulty researchers have resorted to multiscale techniques. These techniques relate to the development of elasto-plastic constitutive equations through a micro-mechanic approach within the contact area and homogenization procedures of the formulation so that the stresses at the interface depend on the individual responses of asperities. Such constitutive equations are always derived from statistical models.

These statistical models take into account the probability density function of asperities along the surfaces in contact. These functions can be derived from the topographical information extracted by profilometry. Approximately 100 variants to evaluate the surface roughness can be involved, but in dentistry one of the most commonly used parameters to analyze the topography is the average roughness (Ra), defined as the arithmetic mean of the amplitudes found in a profile. Nevertheless, the Ra parameter does not provide any other information about the texture features [6, 10].

Most of these contact models assume a normal distribution of asperity heights [11, 12, 13], which may not represent the enamel roughness [14, 15]. In this case, a combination of skewness and kurtosis could be useful to describe the shape of the topographical height distribution and its effect on friction behavior [16]. Skewness is the measure of the asymmetry of surface deviations with reference to a mean plane; and kurtosis is the measure of the peakedness, or sharpness, of the height distribution topography. In a Gaussian distribution of topography, skewness is equal to zero and kurtosis is equal to three. Distributions flatter or peakier than the Gaussian are referred to as platykurtic and leptokurtic, respectively.

The objective of this work is, from surface texture parameters, to work with analytical and numerical constitutive models for the analysis of contact to identify the influence of these parameters, particularly the skewness and kurtosis, on the homogenized properties of human dental occlusal contact.

2. Materials and Methods

The evaluation of the topography of a surface does not only mean the measurement of profiles, but assigning numerical parameters to provide the user with information that is universally acceptable and meaningful about it. The selection of surface parameters must be made bearing in mind that they

must reflect the distinction between two different surfaces and be sensitive to the properties under study, for example with respect to wear. For this work we selected the following three-dimensional texture parameters:

Sa (μm): average roughness. This dispersion parameter is defined as the arithmetic mean of the absolute surface values above and below the mean plane.

Sq (μm): mean square roughness or standard deviation of surface. It is a more sensitive parameter to extreme values than the Sa . Although they are commonly used in many practical applications, the parameters Sa and Sq do not represent well a surface, mostly because they do not distinguish between peaks and valleys. These parameters can be reasonably adequate to describe only isotropic surfaces, subject of this work. These two parameters are strongly correlated [17].

Ssc (1/mm): quadratic mean curvature of the peaks. The more rounded peaks are, the smaller the value of Ssc .

Ssk : skewness. It characterizes the asymmetry of the surface distribution; correspond to the third moments of the density function.

Sku : kurtosis. It characterizes the flatness of the surface distribution; correspond to the fourth moments of the density function.

2.1. Numerical Asperity-Based Contact Model

A first step in the characterization of tribological properties is the knowledge of the contact forces on solid surfaces in contact. For elastoplastic material, as an analytical solution is not possible, numerical models must be developed to solve the contact problem.

Inspired by the approaches proposed by Tworzidlo et al. [18] and Akay [19] for interfaces contact models based on asperities, the following steps are taken:

- Determination of parameters of average roughness Sa , mean square roughness Sq and quadratic mean curvature of the peaks Ssc ;
- Calculation of the probability density function $\phi(z)$ for distribution of the asperities z ;
- Axisymmetric modeling of a number of asperities, called main asperities, with different heights z_i , adopting, according to the random representation of the surface, a hill cosine for the asperities shape [18]:

$$z(x, y) = z_i \cos(xK) \cos(yK) \quad (1)$$

where K is the mean curvature of asperities, taken as Ssc at this work.

- Finite element analysis of micro-contacts between each main asperity and a rigid plane, as an analogy to a Hardness test, where the tip of the penetrator is almost flat;
- From the micro-responses $X(z_i, K)$ obtained in the previous stage (where X can be contact force or real contact area), the values for homogenized macro-contact $E^*(X)$ expected at the interface is estimated by numerical integration of:

$$E^*(X) = N \int_{-\infty}^{\infty} X(z_i, K) \phi(z_i) dz_i \quad (2)$$

where N is the number of asperities at the interface, and $\phi(z_i)$ are the frequencies of each main asperity with height z_i in contact with the rigid plane.

- Estimation of homogenized surface hardness as the ratio between overall resistance force and real contact area and the homogenized yield stress, using a ratio between overall contact pressure and indentation;

To evaluate the influence of surface topography in the response to human dental occlusal Contact, four situations were hypothesized. In the first case, it was considered a constant mean curvature for all surfaces and the mean roughness was varied. In the following case, the mean roughness was fixed and the mean curvature of the asperities was varied. In both cases the spacing between peaks was maintained and it was assumed a normal heights distribution of the asperities z :

$$\phi(z) = \frac{1}{Sq\sqrt{2\pi}} \exp \left[-\frac{(z - Sa)^2}{2Sq^2} \right] \quad (3)$$

The strong correlation between the two amplitude roughness parameters was admitted, given $Sa = Sq$. The following ranges were tested, based on findings in the literature [20, 15, 14], for the first two surface texture parameters considered in the analysis:

- $0.1 \mu\text{m} < Sq < 1.0 \mu\text{m}$ with intervals of $0.1 \mu\text{m}$;
- $0.07 \mu\text{m}^{-1} < Ssc < 0.25 \mu\text{m}^{-1}$ with intervals of $0.018 \mu\text{m}^{-1}$;

For the next two cases the Pearson system of frequency curves was used to generate probability density functions of different skewness and kurtosis values, inspired by the approach proposed by Tayebi and Polycarpou [16]. The Pearson system of frequency curves is a family of curves that can generate a density function that models the roughness of a given surface if its first four moments are known, i.e., the mean, standard deviation, skewness and kurtosis [18].

To study the skewness effect, the generated density functions have a fixed kurtosis value of three, while the skewness is varied from -1 to 1 . In the second set, the skewness is fixed at zero, and the kurtosis is varied from 2 to 20 , corresponding findings in the literature [20, 15, 14].

2.2. Axisymmetric Numerical Models

For each surface, the domain of the probability density function was divided into 25 intervals to represent the main asperities. In this analysis the material was considered isotropic elasto-plastic.

A finite element analysis of micro-contacts between each main asperity and a rigid plane was performed (axisymmetric models), simulating a micro-hardness test, imposing an indentation of $0.3 \mu\text{m}$ (the same order of magnitude of instrumented hardness test).

Below each asperity, a sub-fraction of the material surface is constructed with the same physical properties and depth of $20 \mu\text{m}$. Unstructured mesh with linear triangular elements (under the slope of the asperity) and linear quadrangular elements (in the sub-surface of the material) were generated. The elements were smaller as it approached the contact regions (average size of about $0.25 \mu\text{m}$) as can be seen in Fig. 1.

The contact was solved by Lagrange method, without considering the friction force, as at this scale the roughness are considered smooth. The rigid plane was selected to be implemented with master surface elements, while asperities received slave surface elements. The plane was displaced vertically down by small fixed increments ($0.01 \mu\text{m}$) to achieve a total displacement of $0.3 \mu\text{m}$. The “force-separation” and “area-separation” curves were monitored at each increment.

Recorded data was processed by scripts in Python in order to calculate the contribution of each micro-contact, depending on the frequency of its asperities $\phi(z_i)$, for the expected total response of the interface $E^*(X)$, obtaining the numerical integration of Eq. (2).

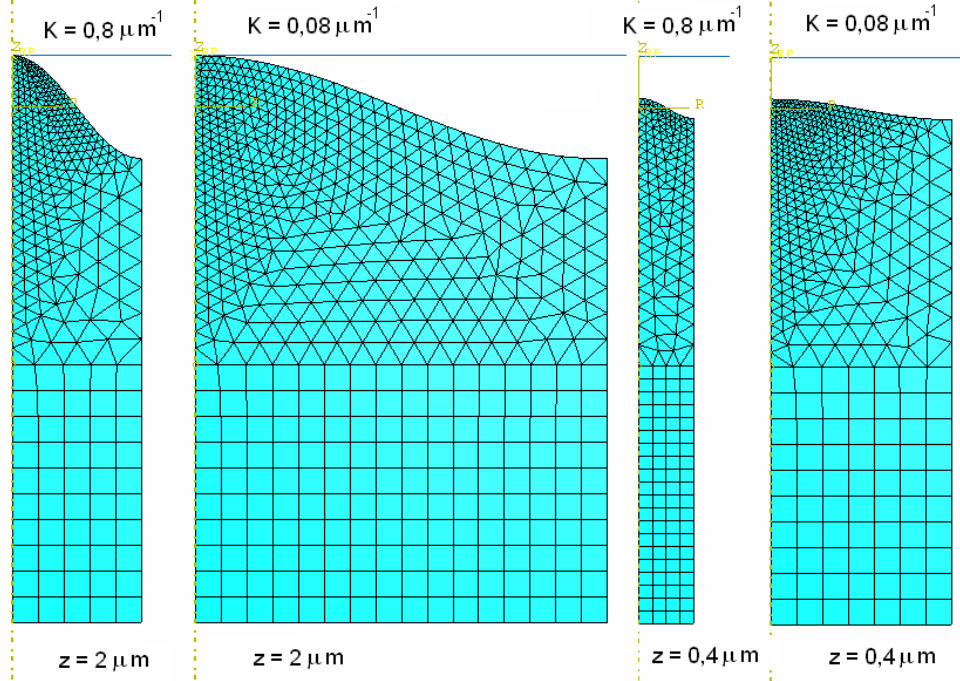


Figure 1: Axisymmetric models used in the analysis.

2.3. Parameterized Scripts Based on Statistical Contact Models

The ABAQUS/CAE[®] is a preprocessor that generates the data entry that contains the geometry, material properties, boundary conditions, applied load and finite element mesh defined by the user. This same module is also a post-processor that provides a graphic display of results.

The graphical user interface (GUI) of ABAQUS/CAE[®] module was used to create a model example of contact between an asperity and a rigid plane, and the commands are issued internally by ABAQUS/CAE[®] after each operation and recorded in a script .jnl file in Python, a object-oriented programming language. This file was accessed and parameterized according to the variables of the problem, mainly to include a loop to repeat the modeling tasks and access the data output for each main asperity considered.

The modification begins with the input of necessary parameters for the analysis: the average roughness, root mean square roughness, the mean curvature and the cell number of numerical integration. The probability density

function of asperities is calculated for the mean roughness concerned and, as a criterion of tolerance, the maximum and minimum height of asperities are found and, based on the number of cells, the integration step is determined.

The loop to cycle through all the main asperities starts and a specific name is assigned to the output file, according to the example:

```
jobName = 'sampleCP_'+str(L)
```

where L is the loop counter.

A function to assist in the automated generation of geometry based on the texture parameters was defined, which calculates a list of the coordinates of np points, located on the asperity slope, which will pass through a spline. The function is:

```
def COSSIN(x):
    result = []
    for i in range(x):
        abs = i * delta
        cordn = C*cos(k*abs)
        z = ( abs , cordn )
        result.append(z)
    return result
```

```
t = COSSIN(np+1)
P = t[(np)]
```

where C is the height of asperity, k is its curvature, and δ is the distance between the points.

The script contains all native commands of Abaqus/CAE module, but parameterized. The contact forces and areas for each increment are accessed from the database output and written in the form of a report (.rpt).

After recording all reports, a routine, also in python, is responsible for reading them successively, calculating the expected total values for the interface, taking into account the contribution of each main asperity. Using the library matplotlib, the final curves are plotted.

3. Results and Discussion

The influence of mean roughness and mean curvature for hypothetical surfaces with normal distribution and the influence of skewness and kurtosis

for hypothetical surface with non-normal distribution on the homogeneized results of real contact area and contact pressure are shown in Figs. 2 to 6.

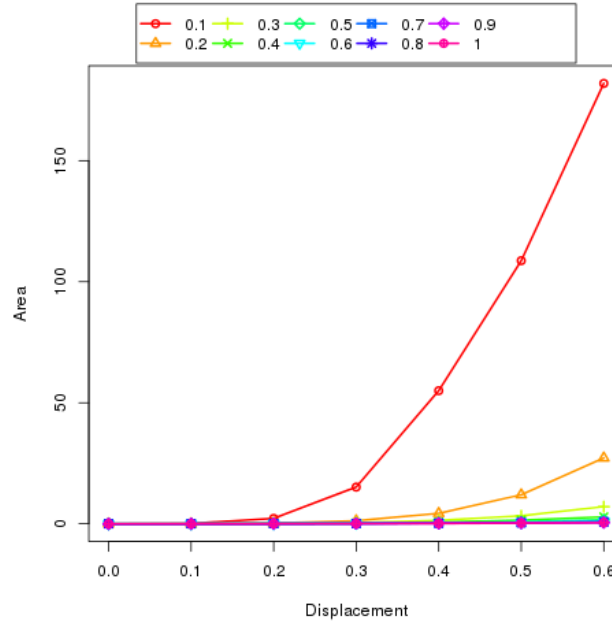


Figure 2: Homogenized contact area versus indentation depth for different mean roughness.

For hypothetical surfaces with normal distribution, the lower the mean roughness, the greater contact areas generated for the same indentation. A surface with low mean roughness will be flattened, offering greater resistance to indentation. The influence on the contact area will also be more significant for lower mean curvature. It can be observed in Fig. 2 that from the mean roughness equal to 0.4, there is practically no difference in behavior between the different hypothetical surfaces.

For hypothetical surfaces with non-normal distribution, different patterns were observed in relation to negative and positive values for skewness. For negative skewness, the higher the skewness, the lower the contact area. From the negative skewness value of -0.6 the influence to the area becomes small. For positive skewness, the opposite is observed, the larger the skewness, the larger the contact area. In this case, the influence is significant for all values.

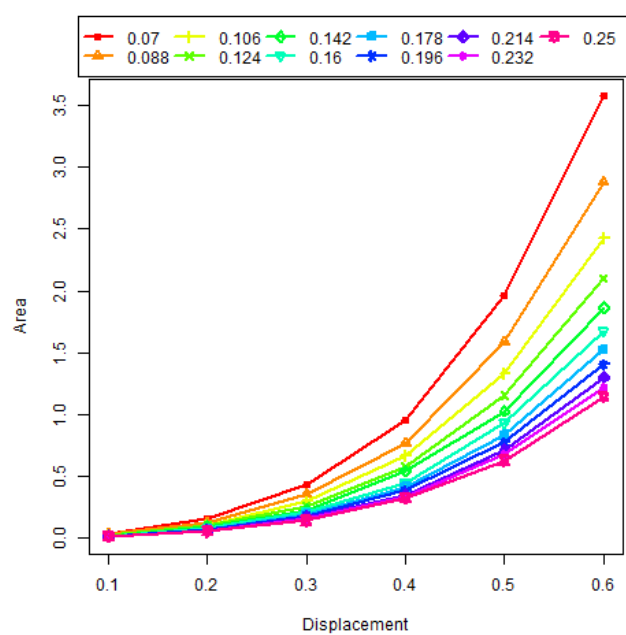


Figure 3: Homogenized contact area versus indentation depth for different mean curvature.

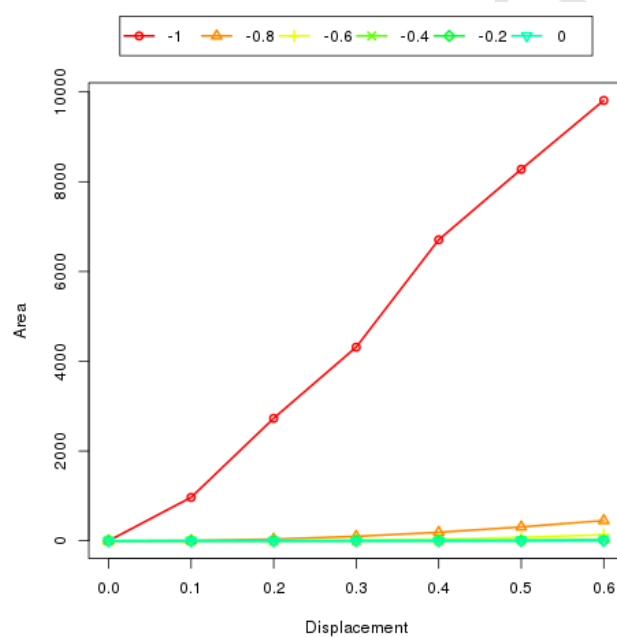


Figure 4: Homogenized contact area versus indentation depth for different negative skewness.

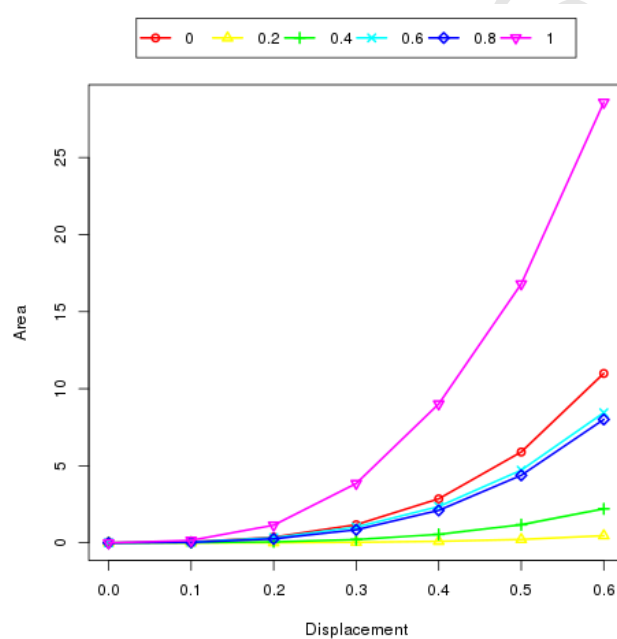


Figure 5: Homogenized contact area versus indentation depth for different positive skewness.

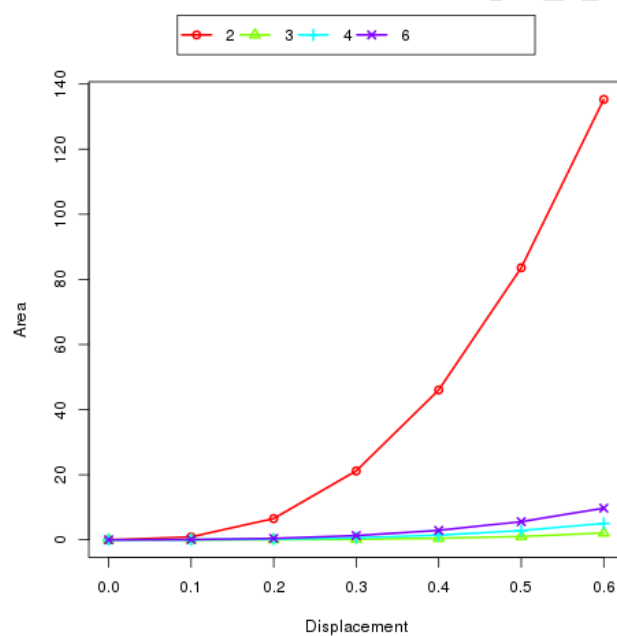


Figure 6: Homogenized contact area versus indentation depth for different kurtosis.

However, the skewness of zero, indicating a symmetrical surface, does not fit to this behavior.

Regarding the kurtosis, two patterns were observed. The first one is related to the unique tested value of kurtosis less than 3. For kurtosis of two, there was a very big influence, because the area found were much larger than for the other values of kurtosis. For kurtosis values from 3, the higher the kurtosis, greater the area.

The relationship F/A , where F is the homogeneized contact force and A is homogeneized contact area may be regarded as a measure of hardness if the micro-contacts are seen as small indentation tests, and was found practically linear in all scans. Based on this analogy, the slope of the curve shows a homogenized hardness, practically constant, of 4.0 GPa, can be seen as an example in the Fig. 7

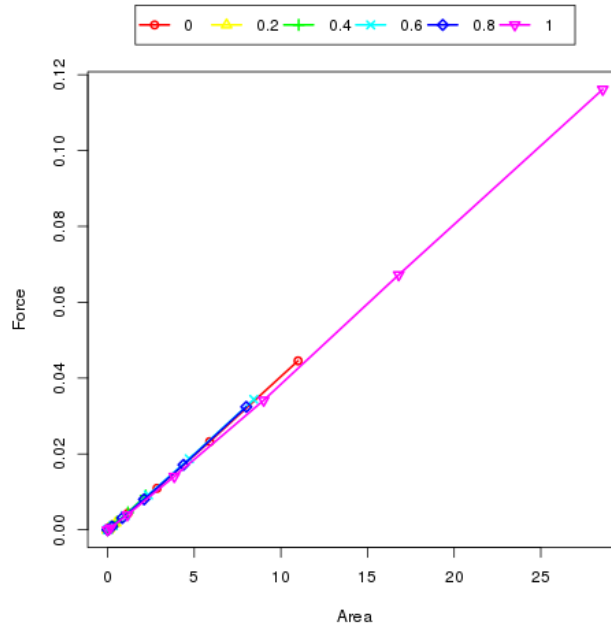


Figure 7: Homogeneized contact force versus homogeneized contact area for different positive skewness: a measure of homogenized surface hardness.

One possible measure of homogeneized yield stress can be obtained by relating the homogeneized contact pressure with the indentation depth. As

for the actual contact pressure, it is observed a transition from a non-linear curve without yield level for lower mean roughness to a curve that looks like perfectly plastic behavior to higher mean roughness as shown in Fig.. Since the other tests were made to the same roughness value equal to 0.5, to which the plastic behavior is already evident at the contact pressure curve, the variation of the yield stress is less noticeable. Still, it can be said that the influence of skewness of negative values is predominant in relation to positive values, as well as the kurtosis.

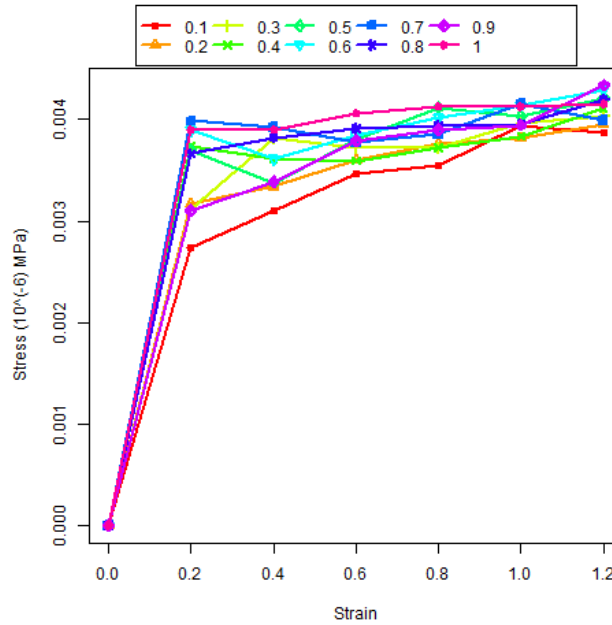


Figure 8: Homogenized contact pressure versus indentation depth for different mean roughness

According to the hypothesis that the friction coefficient for rough surfaces arises from the strain energy, related to the contact pressure, the numerical result is consistent with [21], who conducted experiments in order to isolate the influence of (i) the mean roughness of surface tools and (ii) the difference in materials strength of the pairs on the tribological overall friction behavior and found that friction is sensitive to both. The roughness tested ranged from $0.1 \mu\text{m}$ to $0.65 \mu\text{m}$. These authors observed that the smaller the rough-

ness, the lower the coefficient of friction in the contact interface of tribological pairs. It is also consistent with Pottirayil, Menezes and Kailas [20], who claim that the greater the curvature of the asperities greater the damage during indentations, if we think that the damage relates to the contact pressures. These authors also suggest that, when the contact is predominantly elastic, the friction coefficient increases monotonically with increasing surface roughness, but when the contact becomes fully plastic, the friction force remain unchanged.

By assuming that the friction force is proportional to the real area of contact, the two key parameters used to characterize the asymmetry and the flatness of the surface distribution, the skewness and kurtosis, has a more significant effect on the contact parameters, since its influence leads to different behavior patterns depending on the range in which the parameter is, if positive or negative for skewness and if greater or less than 3 for kurtosis.

4. Conclusions

The mean roughness and the mean peaks curvature of a Gaussian surface influence their tribological behavior. As the mean roughness or mean curvature increases, the nature of the contact changes from elastic to plastic and the friction coefficient increases and becomes saturated. For negative skewness, the higher the skewness, the lower the contact area. For positive skewness, the opposite is observed. The higher the kurtosis, greater the area, except for kurtosis less than 3. The surface hardness is not affected by any of the surface texture parameters tested.

In recent decades, commercial finite element programs for the numerical simulation of mechanical processes became sophisticated and computational efficient, but its strength remains critically dependent on issues such as friction, which are not fully understood. The analysis of tribological surfaces through realistic numerical models, taking into account also material nonlinearities remains a challenge. However, benefits and versatility of numerical methods and the fact that they take into account the deformation analysis in micro-scale points of contact can provide useful information for construction of hypotheses about the phenomenon in investigation. It is recognized that lubrication is not included in this preliminary work. Further verification using experimental data can encourage dentists to become more familiar with computer simulation so that mutual cooperation leads to a better understanding related to contact, friction and wear of dental surfaces.

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