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**Computational Mechanics Framework for Simulations and
Prediction of Wear in Frictional Contacts**

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To the world

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Abstract

A computational finite element modelling of a mechanical model to predict wear, including friction, is proposed in this work. As an expansion of the interface finite element with an embedded profile for joint roughness (MPJR interface finite element), it is designed to solve the frictional contact problem between rigid indenters of any complex shape and elastic bodies. In the formulation, the non-linearity due to contact is considered for predicting contact traction, frictional effects, and wear. This formulation interfaces with FEM software and can embed roughness or general deviations from the planarity as a correction to the normal gap function. The model employs a regularized version of the Coulomb friction law for the tangential contact response while introducing a penalty approach in the normal contact direction. The present framework enables the comprehensive investigation of the tangential and normal tractions via the computation of displacements and the displacement gaps in the model. These tangential and normal tractions can be used to calculate the wear rate via the wear law. The model defines wear by contact force and gaps. Due to this, contact pressure develops wear and the normal gap changes. Model parameters related to the constitutive equations of the interface where two bodies come in contact: regularized coulomb friction law and Archard's wear law outlined. In conclusion, this model predicts the wear and wear rate at the micro-scale level and explains how to formulate and predict wear at the macro-scale level.

Chapter 1

Introduction

My 3-year-old daughter picked up the nail file and rubbed it against the floor and the wooden wardrobes. "What are you doing? Stop it!!!" shouted my wife from a distance. I quickly intervened to explain to my daughter what the nail file was for. I said, "When you rub this on any surface, it will erode, eventually leading to damage. Use this to remove nail polish from your nails." My daughter nodded with a smile.

People have yet to come across wear and friction in their daily lives. From nail polish to aeroplanes, everything undergoes the process of wear. Whether it is your bicycle's tyres, the wardrobes in your home, the footwear you wear, or the clothes you have, nearly all our mundane actions involve friction, resulting in wear.

Friction is the force that opposes the relative motion of the surfaces in contact, while wear is the gradual removal of material from a solid surface.

Wear is a pivotal yet often overlooked phenomenon in the extensive engineering domain. Wear refers to the gradual loss of material or degradation when two surfaces come into contact and undergo relative motion or pressure. Although wear may seem natural on surfaces, the consequences are far-reaching, often called an "iceberg" of the associated maintenance costs. At the core of every mechanical system, from the intricate gears of industry to household appliances, there is susceptibility to wear-induced degradation, known as "wear and tear." The ramification of wear extends beyond mere inconvenience and can cause catastrophic severe failures, expensive repairs, and unplanned downtime, resulting in a loss of productivity, reduced process efficiency, and yield.

I am reminded of my time as a maintenance engineer in the biscuits manufac-

turing industry in Kanpur, India. The primary maintenance issue in the systems was due to wear of the belt and pulley. The sides of the pulley usually wear out over time and often require replacement. Furthermore, the leaf springs used on the sides of the pulley begin to wear out, leading to crack initiation and eventual shut-down. In general, wear can arise from mechanical or chemical causes. Wear related to processes such as fatigue and creep can be devastating.

The detailed consequences of wear can be listed as follows:

1. **Performance Degradation:** Wear manifests as a gradual deterioration of surfaces, leading to reduced performance. Increased friction decreases system efficiency in the absence of lubricants. In precision-focused industries such as automotive and aerospace, shifts in machine component tolerances compromise system functionality and may lead to damage.
2. **Reliability and Durability:** Wear undermines the longevity and reliability of mechanical systems by eroding their structural integrity. Bearings lose smooth rotation, shafts develop grooves, and seals fail to maintain integrity, decreasing reliability. Even slight wear hinders reliability in critical aeroplane applications and requires meticulous attention.
3. **Maintenance Costs:** Wear has a significant impact on the economy, causing unplanned maintenance, repairs, and replacement of worn components. The result incurs direct costs across industries. Moreover, indirect costs associated with downtime and lost productivity further exacerbate the financial burden.
4. **Energy Efficiency:** Friction-induced wear leads to energy loss, resulting in inefficient mechanical systems. The contact area increases as surfaces degrade, leading to additional energy loss. With a growing focus on energy conservation, minimizing wear is a matter of economic impact and environmental responsibility.
5. **Safety Concerns:** Wear-induced failures can pose significant threats, sometimes resulting in catastrophic failures. Worn-out brake pads or tyres can compromise a vehicle's integrity and pose serious safety concerns. Similarly, in industrial settings, worn-out components can pose a severe threat. Understanding and mitigating the risk of wear on time ensures the safety and well-being of mechanical systems.

In essence, wear is not just a byproduct of mechanical interactions but a determinant of system performance, reliability, and safety. By comprehensively understanding the mechanics of wear and coming up with effective mitigation strategies to maintain system performance that underpin engineering practices.

Due to many of the concerns mentioned above, the study of wear is a cornerstone discipline in diverse industries and applications. On the other hand, the study of friction is critical in wear. Furthermore, wear results from the frictional forces that develop in the body. In the following section, the basic friction theory is put forth first, followed by the primary wear mechanism.

1.1 Basics of friction

Friction arises from the microscopic interaction of two surfaces in motion under contact. Friction offers resistance hindering smooth sliding or rolling motion of the contacting bodies. In mechanical systems, friction manifests as resistance to motion, dissipating energy through heat, sound, and light. Frictional forces serve as the driving force for wear processes, initiating material removal, surface deformations, and tribological transformations. In contrast, wear alters the surfaces, influencing friction. Tribology studies these bidirectional interactions and lubrication to reduce friction[1].

The frictional force (F) is the lateral force that acts in the plane of the surface, whose force is proportional to the normal force (N):

$$F = \mu N$$

where the proportionality constant μ as termed a friction coefficient. The friction forces mainly depend on the properties of the bodies in contact and the contact area.

Due to the intrinsic nature of surface area dependency, the precise computation of the frictional forces presents several challenges related to surface roughness, unevenness at multiple length scales, and chemical composition. For these reasons, a micro-scale analysis of the friction becomes necessary. The microscopic system that can generate friction can be mainly categorized as:

1. Adhesion;
2. Mechanical interactions of surface asperities,
3. Plowing of one surface on the other;

4. Deformation or fracture of surface layers such as oxides;
5. Intrusion and local plastic deformation from third bodies.

See [1] for a more detailed review of friction.

1.2 Wear

Consider an example of a protective film on a hard surface, such as a screen protector on a phone. When the protective film on hard surfaces fails, it can cause damage due to rubbing between the two surfaces. This damage can result in severe wear and tear. If the film fails and the two surfaces stick together, it is called 'adhesive wear.' On the other hand, if the film contains hard particles or rubs against one surface without protection, it leads to a type of wear known as 'abrasive wear'. In some cases, the protective film is weakened by chemicals from the surfaces it is meant to protect. As a result, "corrosive wear" occurs, providing some lubrication but still causing significant wear. When atmospheric oxygen causes the breakdown of the film, it's called 'oxidative wear'. Other types of wear are caused by fatigue, erosion, impact, and fretting. Still, this study will focus on adhesion, abrasion, and corrosion wear due to their significant impact [2].

1.2.1 Adhesive wear

Adhesive wear is a severe form characterized by high wear rates and a sizeable uneven friction coefficient. Sliding contacts can be quickly damaged by adhesive wear, and in severe cases, sliding motion may be prevented by very high coefficients of friction or adhesion. Increasing the surface roughness or hardness of the contacting bodies can reduce adhesive wear. [2, 3]

The oxide film, which may only be a few nanometers thick, prevents proper contact between metals and inhibits severe wear unless intentionally removed. In vacuum experiments [2], it has been observed that as surface contamination is reduced, the adhesion between the metallic surfaces becomes very strong.

In all cases, the adhesion or separation force is greater than the contact force. The tendency to adhere does not depend on the solubility of metals or their atomic size. The highest adhesion occurs in a combination of like materials, such as iron to iron, but many other combinations of different metals also show relatively high adhesion. Many tests on various metal mixtures have revealed that when there is strong adhesion, transfer of the weaker metal to the more substantial metal occurs.

Every metal strongly tends to stick when in contact with another solid. However, there are significant differences between specific elements. Metals mainly exist in four main types of crystal structure: face-centred cubic, body-centred cubic, hexagonal close-packed, and tetragonal. It has been experimentally established that metals with a hexagonal close-packed structure exhibit much less bonding than other crystal structures [2, 1]. The metal's high hardness, sizeable elastic modulus, and surface energy also inhibit bonding. The coefficient of adhesion against hardness for pure metals shows essential differences in bonding between metals of similar hardness but different crystal structures. Hexagonal close-packed metals contain far fewer slip systems and are, therefore, less ductile than face-centred and body-centred metals, resulting in lower bonds.

In summary, the transfer of electrons between metals allows an adhesive solid connection between two similar or dissimilar metallic elements. A preventive factor in adhesion is the minimum load that causes plastic flow and, therefore, the occurrence of precise contact between surfaces.

In numerous experimental investigations [2, 3, 4, 5], it has been observed that metals and polymers can also exhibit a high degree of adhesion. The adhesion examined between a tungsten surface and polymers such as polytetra fluoroethylene and polyimide is strong enough to cause the transfer of polymer to the metallic surface while the two materials are in contact. The strength of adhesion is related to the presence of reactive non-metals, such as fluorine, in the polymer. The surface atoms of the polymer are supposed to bond with the surface atoms of the metal, which can occur regardless of the inertness of the polymer in bulk. Most polymers adhere to other materials by van der Waals forces, which are not strong enough for material detachment in most wear cases.

Under appropriate circumstances, relatively strong adhesion between metals and ceramics can occur. It has been observed that only metals that do not form even oxides show low friction coefficients against ceramics. Metals generally have lower strength than most production ceramics, so on the break of the adhesive contact, metal fragments are left adhering to the ceramic to form a transfer layer. The adhesion of ceramics to metals is reduced by surface contamination, similar to that seen with metal-metal contacts.

If adhesive wear is allowed to advance unchecked, various unwanted consequences can follow, including elevated friction with the potential transfer of particles leading to damage. In some cases, transfer particles can jam the sliding contact. Another problem caused by adhesive wear is a very high wear rate and severe sur-

face damage. Experimental results have shown an increased likelihood of wear particle production due to the roughness of contacts during adhesive wear compared to, for example, abrasive wear.

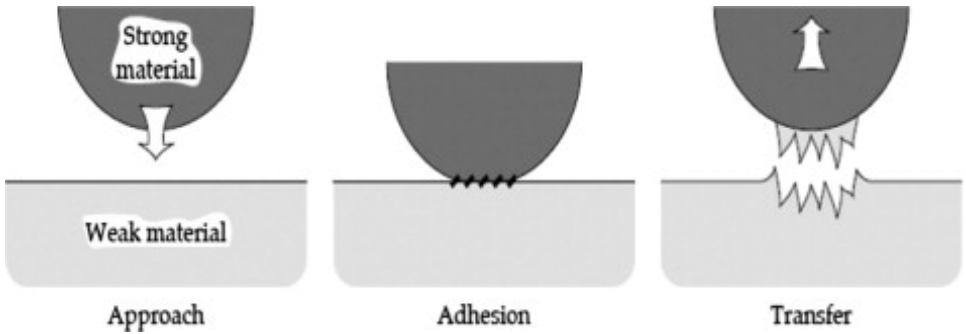


Figure 1: Mechanism of metal transfer by adhesion[2]

1.2.2 Abrasive wear

Abrasive and erosive wear are forms of wear that occur when hard objects come into contact with particles. Abrasive wear involves material loss due to solid particles rubbing against a surface [2], while erosive wear is caused by particles impacting a hard surface. Cavitation is another form of wear that happens when bubbles in a fluid hit a surface. Abrasion and erosion are rapid and severe types of wear and can result in significant costs if not correctly managed[6]. Abrasive wear occurs when a hard object rubs against particles of a substance with similar or greater hardness. For example, the wear of shovels on earth-moving equipment is a typical example related to abrasive wear. Even a primarily soft material can cause abrasive wear if hard particles are present. For example, silica in plant fibres can cause abrasive wear on cane cutters and shredders when working with natural materials like sugar cane.

Mechanism of Wear: Initially, it was believed that abrasive wear by grits or solid roughness resembled cutting by a series of machine tools. However, microscopic examination reveals that the cutting process is only approximated by the sharpest (largest) grits, and several other indirect mechanisms are involved. The particles or grits may remove material by micro-cutting, micro-fracture, pull-out of individual grains [3], or accelerated fatigue due to repeated deformations as shown

in Fig. 2. The cutting process represents the classic model where a sharp grit or solid roughness cuts the softer material, as shown in Fig. 2(a). The worn material may be fragile, and the worn surface can fracture, as in Fig. 2(b). Cutting is unlikely when a blunt grit abrades a malleable material, and the worn surface continually deforms, as in Fig. 2(c). The fourth mechanism involves grain pull-out and applies mainly to ceramics where the boundary between grains is relatively weak, as in Fig. 2(d) .

Abrasivity of Particles: A particle or grit is typically considered abrasive if it can cause fast abrasive wear. In most cases, the hardness of the material must be less than 0.8 of the particle hardness for fast abrasion to occur [2]. It has been observed that some abrasive wear and damage to a surface still occur unless the yield stress of the material exceeds that of the abrasive particle [3]. Prolonged abrasive wear continues until the hardness of the abrasive and worn material is equivalent. Their hardness primarily determines the resistance of materials to abrasive wear. It is widely recognized that hard materials exhibit slower abrasive wear rates than softer materials. Consequently, hard materials such as ceramics exhibit good abrasive wear resistance.

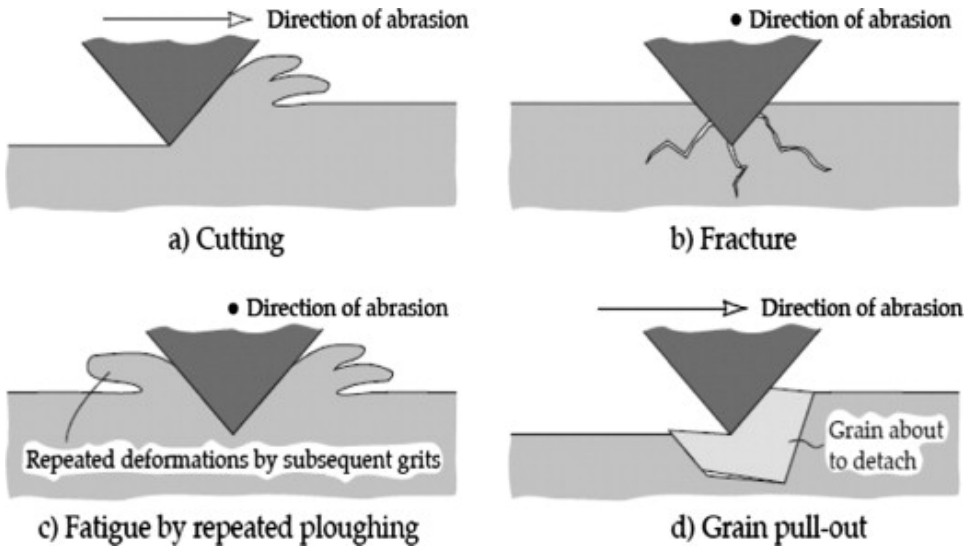


Figure 2: Mechanisms of abrasive wear, a)micro-cutting, b)fracture, c)fatigue and d)grain pull-out[2]

The impact of temperature on abrasive wear can be categorized into two main

effects. First, the influence of elevated ambient temperature on abrasive wear has been minimally studied due to experimental complexities. Some tests on the abrasive wear of copper and aluminium showed a slight increase in wear at temperatures up to 400 °C for copper and no effect for aluminium. Additionally, as the temperature increases, there is a corresponding decrease in the hardness of both the worn material and the abrasive grit. This trend has been observed in experiments conducted with temperatures up to 2000°C, where most metals, metallic carbides, and nitrides showed a similar decline in hardness with increasing temperature. See [7, 8]for more details. Temperature effects on abrasion under high-temperature conditions are demonstrated in Fig. 3.

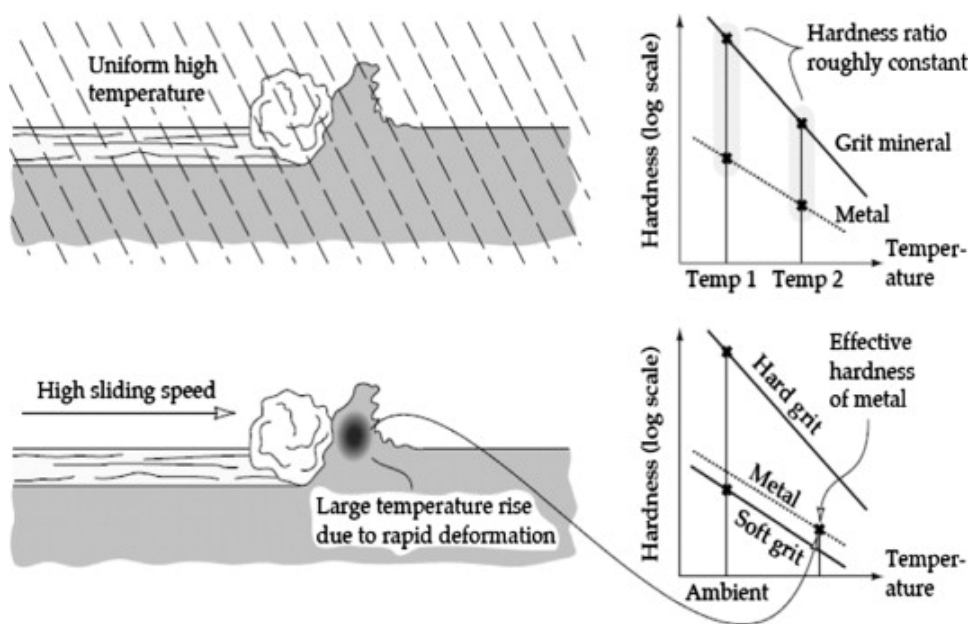


Figure 3: Temperature effects on abrasion under uniformly hot conditions and under high rates of frictional energy released during rapid abrasion[2]

Second, the temperature increase caused by plastic deformation by abrasion is associated with high grit speeds. Dynamic thermo-couple measurements with an electrically conductive abrasive revealed that temperatures as high as 1000°C can be reached during abrasion. Unlike the temperature increase induced by elevated ambient temperature, in the case of plastic deformation through abrasion, the grits

remain relatively cold due to the transient nature of abrasion. Moisture also significantly impacts abrasive wear rates[1].

Generally, abrasive wear rates increase with moisture content in the atmosphere, although there are instances where the opposite occurs[6, 9, 10]. Predicting the specific impact of moisture is challenging, as the humidity can either sufficiently weaken the grit to create a more significant number of new cutting edges or cause grit disintegration into non-abrasive, fine particles. The worn material may also be affected by humidity, increasing or decreasing the abrasive wear rates, depending on the specific abrasive and worn materials involved. In summary, abrasive wear can be controlled or mitigated by increasing the hardness of the worn surface to at least 80%

1.2.3 Corrosive wear

Corrosive and oxidative wear occur in many situations, both in lubricated and unlubricated conditions. These types of wear occur due to a chemical reaction between the worn material and a corrosive medium, which can be a chemical reagent, an inadequate lubricant, or even air. Corrosive wear is a general term for any type dependent on a chemical or corrosive process, while oxidative wear refers to wear caused by significant oxygen exposure. An attractive characteristic of both types of wear is that a reduced coefficient of friction often accompanies a high wear rate[2].

Corrosive wear mechanisms surface chemical reactions that help prevent adhesive wear can significantly deteriorate the base material. If a metal corrodes to form a film on its surface while being subjected to sliding contact, one of the following four processes may occur [11]:

- A lubricating solid film may be formed, inhibiting corrosion and wear.
- Depending on the sliding contact, a weak film may develop with a short lifespan under the sliding contact. In this case, the friction coefficient may or may not be low. The protective surface films may wear off, and a galvanic coupling between the remaining films and the base substrate may result in rapid corrosion of the worn surface area.
- The corrosive and wear processes may occur independently, leading to material degradation, which is simply the sum of these two processes combined.

These hypothetical forms of corrosive wear are illustrated schematically in Fig.

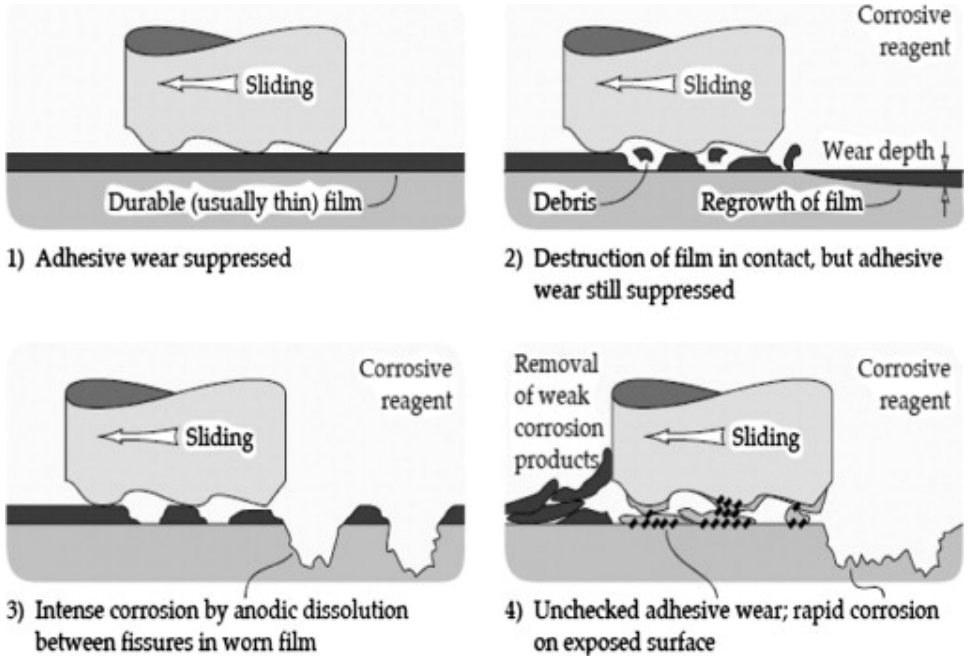


Figure 4: Models of interaction between a corrosive agent and a worn surface[2]

1.3 Thesis overview

PCD samples used to conduct the experiments are of industrial quality. Specifically, Grade 820 is used as a tip of the drilling machine cutting the rocks, whereas Grade 600 is used for cutting hard materials, including metals. The PCD samples produced in the industry differ from the experimental results available in the literature. Consequently, it is crucial to accurately describe the industrial-grade material microstructure along with the wear profiles. Regarding the PCD experimental results available in the literature, the roughness and the profilometer results are rare. Even if it exists, it is random, and the exact material description, including the properties, is unavailable. Hence, the characterization of the material is complex. The experimental results aim to characterize the industrial-grade PCD samples and understand their microstructure completely. Furthermore, estimate the life of this material. To maintain confidentiality and honour the nondisclosure agreement, only small parts of the experimental results are presented in the thesis.

The numerical model aims to present an accurate description of the experimental results. The proposed thesis provides a starting point for a more extended development, which is still in progress. Specifically, the model describes the wear profile in the half slip condition in the static loading. Furthermore, the next step is to consider the full slip condition, followed by combined horizontal and vertical loading. This model will be further extended to include the roughness in both the cutting and the substrate profile via statistical analysis of the roughness profile.

Furthermore, a micro-mechanical analysis will be included to accurately describe the material behaviour in full slip condition. Moreover, the model will be extended to include fatigue loading, consequently leading to the estimation of the lifetime of the PCD samples. Within this context, Hilti Schaan is also interested in understanding the fracture behaviour in these materials. Ultimately, the full slip fatigue model will be extended to include the fracture via Phase-field methods to fracture. Considering the long-term efficiency of the mathematical model, variational methods to wear are proposed in this thesis as a first step.

In the remainder of the thesis, Chapter 2 presents the experimental results conducted at Hilti-AG. Section 2.1 briefly introduces the tested polycrystalline diamond (PCD) material, its advantages, and disadvantages. It also discussed the procedure and importance of the test, along with the details of the experimental setup. Section 2.2 gives the details of the types of specimen, its grade, characteristics and the size of the specimen. Furthermore, it also presents information on the surface topology of the specimen by showing the specimen's SEM, EDX, and volume fraction, providing an understanding of the microstructure and other materials on the surface. Section 2.3 presents the experimental results, showing the effect of surface topology on normal forces and friction force develops at different loading conditions. Wear tracks made on the specimens are discussed here. Lastly, Section 2.4 describes and compares the surface roughness of the samples used before and after the test using the confocal profilometer images and the probability density curve of the samples.

In Chapter 3, theoretical and computational aspects related to the numerical computation of the wear are presented. Specifically, Section 3.1 presents a short introduction to the equilibrium equations in the elastic material. Using energy considerations, the thermodynamic consistency of the balance equations is discussed, followed by a mathematical formulation that includes the prediction of the wear profile. This, in particular, is articulated using variational methods to wear, where governing equations in the strong and weak form are presented. Furthermore,

an interface containing embedded roughness is presented using MPJR embedded roughness theory. A finite element implementation of the wear problem and a detailed discussion of driving forces are presented in Section 3.2.

In Chapter 4, the numerical approximation for wear developed in Chapter 3 is tested using benchmark examples. Specifically, three geometries of similar profiles with cylindrical, flat, and Weierstrass-Mandelbrot (WM) functions as indenters are presented, followed by a detailed analysis for each case. Furthermore, the normal and tangential tractions are used to evaluate the physics, whereas the wear rate for each case is computed. A detailed dimensionless analysis is performed for each case involving tractions, and their behaviour is justified with the contour plots.

Finally, the conclusions are presented in Chapter 5, followed by the future developments within the scope of this thesis.

Chapter 2

Sliding Wear Experiment

This chapter corresponds to the experimental investigation carried out during the six-month internship at Hilti, Schaan, Liechtenstein. Liechtenstein is a stunning Alpine country in the Upper Rhine valley of the European Alps, which borders Austria on one side and Switzerland on the other. The headquarters of the Hilti group is located in the lush green Alps of Schaan. The experiments were conducted under Dr. Steven Moseley, Chief Scientist (Hard Materials) & Key Expert (Inserts Development), and Dr. Carsten Peter, Simulation Expert.

Polycrystalline diamond (PCD) material has revolutionized the cutting tool industry due to its exceptional hardness, wear resistance, and thermal conductivity. PCD is formed by synthesizing diamond particles into a solid composite under high-pressure and high-temperature conditions, with the aid of a catalytic metal[12],[13].

One of the main advantages of PCD cutting tools is the ability to withstand elevated temperatures without losing their hardness. This makes them suitable for high-speed cutting or machining of hard materials such as carbon fibre composites, aluminium alloys, and titanium. The exceptional thermal conductivity of PCD also helps dissipate heat generated during cutting, reducing the risk of tool damage and improving tool life.

Another critical benefit of PCD cutting tools is their remarkable wear resistance. PCD material is rigid and even more complex than cubic boron nitride (CBN) and tungsten carbide. This hardness enables PCD cutting tools to maintain their sharpness and precision longer, resulting in higher productivity and reduced downtime for tool changes. The size of the diamond grain significantly influences the machining performance of the PCD tool[14]. The coarse grade offers greater impact

resistance and fracture toughness, whereas the fine grade possesses higher cobalt content, hardness, and thermal resistance.

The objective of conducting a sliding wear experiment on PCD samples is to evaluate their wear resistance and performance under dry sliding conditions. By subjecting PCD to sliding wear tests, researchers aim to measure the material's wear rate, friction coefficient, and surface damage. In addition to testing different loading conditions, surface analysis techniques such as scanning electron microscopy (SEM) and profilometric acquisition will be used to examine wear mechanisms and characterize the worn surface of PCD material. Moreover, the following sections will present a statistical analysis of the surfaces before and after the experiment. The wear behaviour of PCD under different operating conditions will be analyzed to optimize its performance and enhance its application in industries, including cutting tools, bearings, and wear-resistant coatings.

2.1 Experimental Test Description

To analyze the physical properties of the sample, a destructive measure system test was carried out, called the linear oscillation test device" or TRIBOTEST rig.

The experimental setup consists of a rigid metal cylinder sliding on the PCD sample and lying on a supporting flat rectangular block where the load cell is applied. The Schematic diagram of the tribotest rig is shown in Fig.5. During the test, it is possible to control the sliding motion of the cylinder and the normal force applied during the sliding. The cylinder and the sample surfaces were in contact with a relative sliding (transitional) motion horizontally with no lubrication at the interface.

In Fig. 6, the Tribotest rig drives linearly for the finite displacement of 3.5mm in oscillating motion with a frequency of 5Hz for a run time of 100sec. The cylindrical rigid metal is fixed in the upper part (moving linearly), and the PCD sample is in the lower part. Before fixing, the samples and the cylinder were cleaned with an ultrasonic cleaner and isopropyl alcohol. After every test, the cylinder was washed with isopropanol to remove the particles from the previous test. After fixing the samples, the load is exerted from the load cell, which makes contact between the solids. Three different normal loads, i.e. 350N, 550N, and 1300N, have been applied from the load cell.

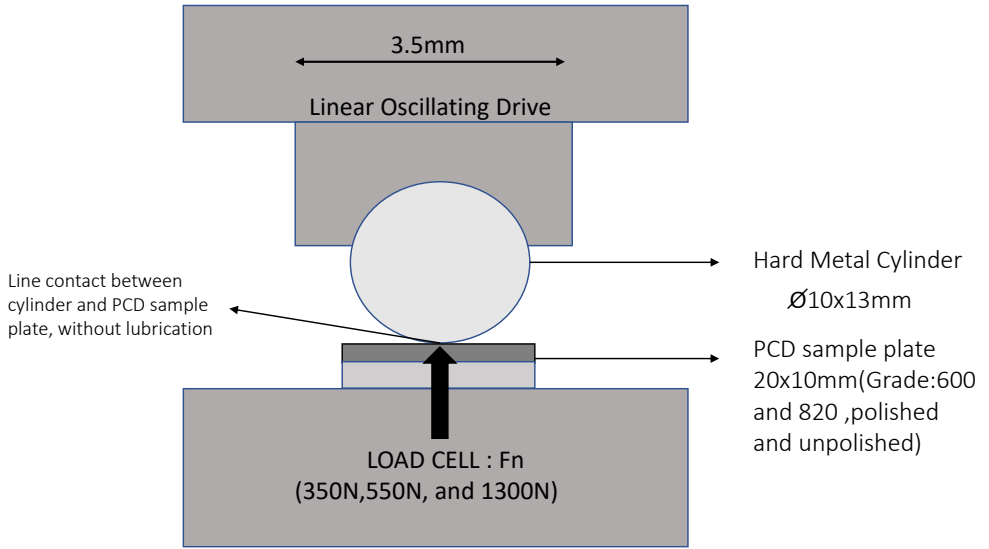


Figure 5: Schematic representation of Tribotest rig

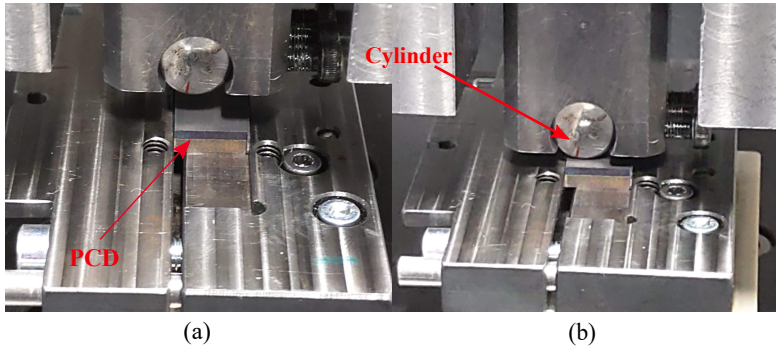


Figure 6: Tribotest rig: (a) cylinder and PCD clamped position, (b) cylinder making contact with PCD

2.2 Material Properties

The size of the tested PCD samples is 20x10mm (see Fig. 7), while the cylinder is 10x14mm. The PCD samples have Young's modulus of 900GPa and Poisson's ratio of 0.3. The cylinder's Young's modulus is 210GPa, and its Poisson's ratio is 0.22.

Four types of PCD samples have been tested: grade 820 polished and unpolished

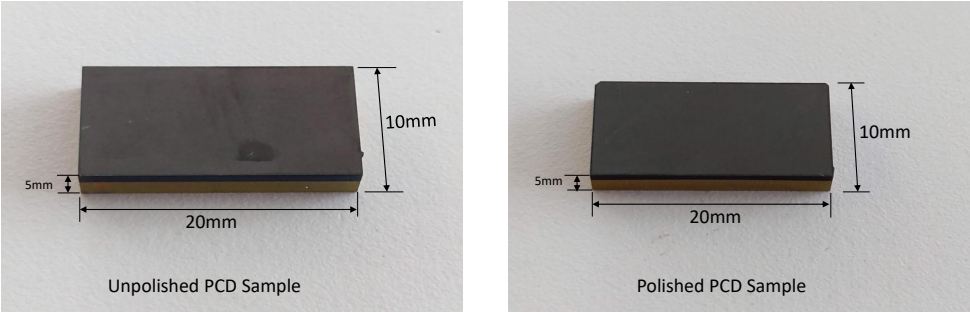


Figure 7: PCD Samples for the Tribotest.

and grade 600 polished and unpolished, considering two samples for each type. The PCD material shows different characteristics according to the grade type, as summarized in Tab. 1. The experiments used eight PCD samples and six stainless steel cylinders, as shown in Fig. 8. Based on the material’s microstructure and composition of the material in the system. The grade names are indexed based on the Hilti policy.

PCD Grade description	Characteristics
grade 600 -Tooling Grade -Designed for Rough Machining	Impact Resistance Extremely High Hardness High Wear Resistance (metal cutting)
grade 820 -Drilling Grade -Percussion/3-Cone Bit Application	Impact Resistance Moderate Hardness High Wear Resistance (high <i>SiO₂</i> rock)

Table 1: Material description

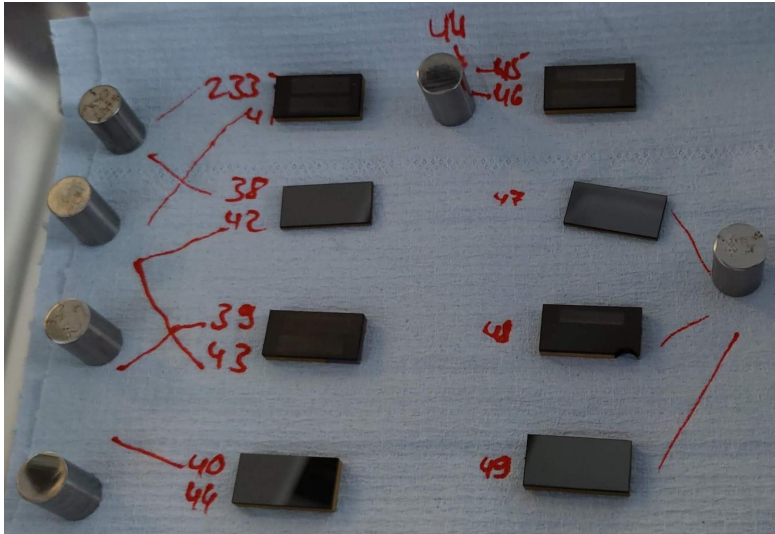


Figure 8: The test has been conducted using 8 different PCD samples and 6 steel cylinders.

2.2.1 Surface Characterization

Scanning electron microscopy (SEM) is a technique that can be utilized to investigate the morphology of samples at greater levels of magnification than optical microscopy, providing insights into the surface topology and composition of PCD materials of grade 600 and grade 820 before experimentation. The SEM analysis was conducted using the Zeiss Supra 40VP model from Electron Microscopy Instruments, located in the Material Testing Lab at HILTI-AG, to gather surface data on the PCD. The SEM images revealed intricate details of the crystal structure and grain boundaries of the PCD materials, highlighting the uniform distribution of diamond particles within the matrix. Furthermore, the elemental composition mapping showed the presence of carbon, nitrogen, and trace amounts of cobalt, confirming the desired properties required for cutting applications in the tooling industry.

Figs. 10 - 13 provide insight into the microstructure of polycrystalline diamonds obtained with the SEM analyses. This study does not include a detailed analysis of the microstructure of polycrystalline diamond. However, future research could focus on a more in-depth examination of the microstructure of polycrystalline dia-

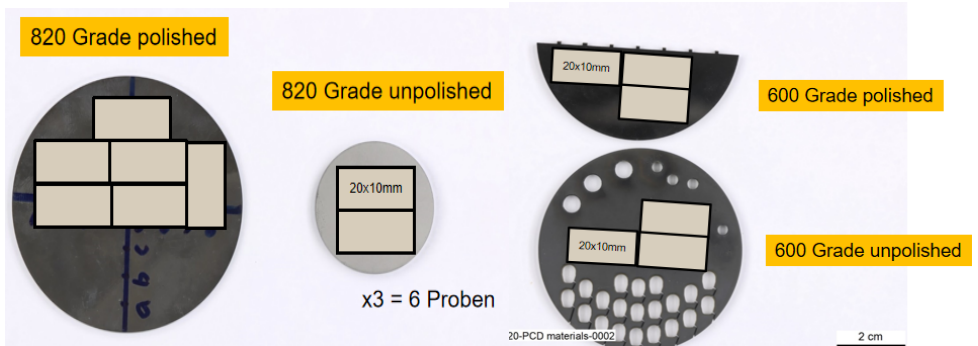


Figure 9: Pattern of Samples preparation of PCD for the SEM test

mond to better understand its properties and potential applications. Fig. 10 refers to the polished PCD specimen of grade 600. Figs. 10(a) and (b) depict the microstructure before the experiment obtained using SEM. Fig. 10 (c) shows the black carbon content of the diamond, as the grain size of the sample is polished and very condensed, the total area fraction is about 83.98% with an area of the object of $0.03mm^2$. Fig. 10 (d) highlights the different amounts of other content present on the surface of the specimen observed through Energy dispersive X-ray analysis (EDX). The white spots in the images show the presence of Tungsten with 80.7% in that particular spectrum, and the black colour shows the majority of the presence of carbon content.

The SEM scanning of the unpolished sample of grade 600 PCD is presented in Fig. 11 (a) and (b). In this case, the micro-structure is not refined, and the grain structure is not visible, leading to less effective cutting and wear resistance. It is crucial to ensure that the polishing process is carried out effectively to enhance the performance and durability of the PCD in various cutting applications. In Fig. 11 (c) and (d), the EDX image shows the surface composition. The results are compared to the polished sample of grade 600; it is visible that, apart from Tungsten (white portion), some other materials or oxides are also present on the surface of the grey portion. Additional materials or oxides on the unpolished surface can compromise the cutting efficiency and wear resistance of PCD grade 600.

The same analysis has been conducted for the unpolished and polished sample of grade 820. Fig. 12 (a) and (b) show the micro-structure of polished grade 820; we can observe the well-defined diamond grains distributed evenly throughout

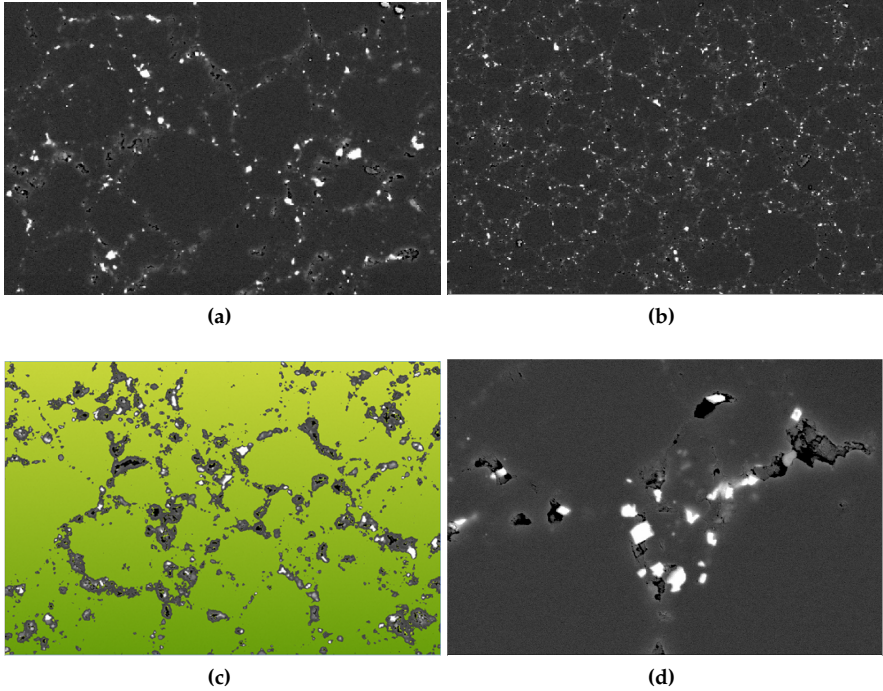


Figure 10: PCD grade 600 polished specimen surface microscopic images before experiment, a) SEM image at $10\mu\text{m}$, b) SEM image at $20\mu\text{m}$, c) volume fraction of the specimen of grade 600, d) EDX image of grade 600.

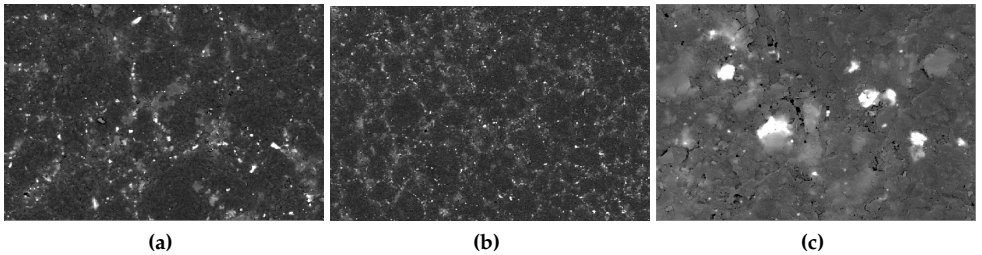


Figure 11: PCD grade 600 unpolished specimen surface microscopic images, a) SEM image before experiment at $10\mu\text{m}$, b) SEM image before experiment at $20\mu\text{m}$, c) EDX image of grade 600

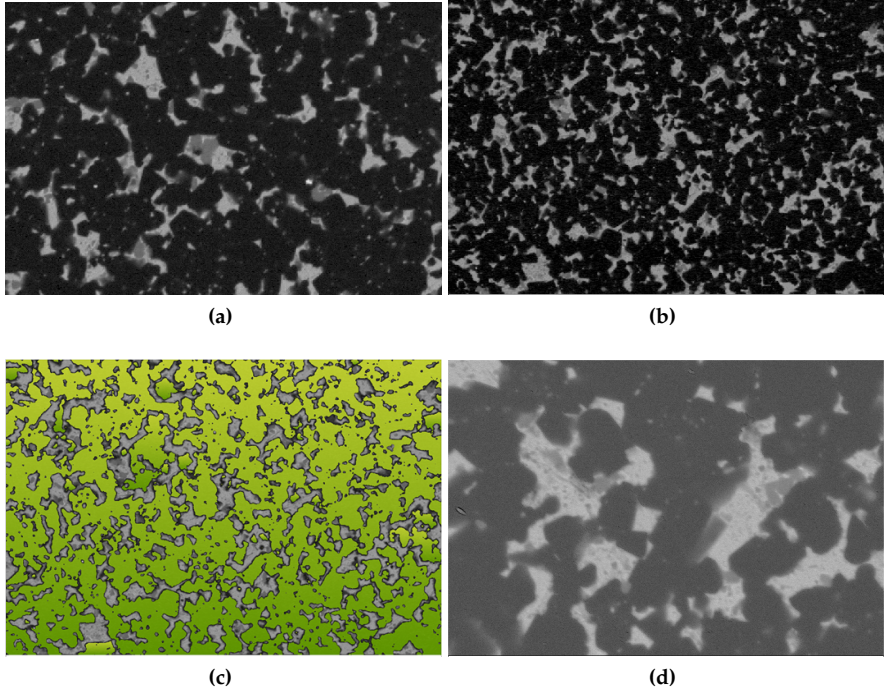


Figure 12: PCD grade 820 polished specimen surface microscopic images, a) SEM image before experiment at $10\mu\text{m}$, b) SEM image before experiment at $20\mu\text{m}$, c) volume fraction of the specimen of grade 820 and d) EDX image of grade 820

the matrix, contributing to the high wear resistance of the material. The uniform distribution of diamond grains plays a crucial role in increasing the hardness and abrasion resistance of grade 820. In Fig. 12 (c), the percentage of the volume of diamond added during the sintering behaviour, the total area fraction is approximately 66.68% with the object area of 0.03mm^2 . In contrast to the grade 600 sample, in Fig. 12 (d), the grey portion shows Titanium (Ti) is also present on the surface with 61.5% in that particular portion. Also, the white colour portion shows a lot of binders like cobalt and Tungsten-carbide, which decreases the hardness of the material.

Fig. 13(a) and (b) show the micro-structure of unpolished grade 820, with Fig. 13 (c) and (d), the white and grey colour portion shows that many binders are present on the surface, reducing the hardness of the material at the surface. The mi-

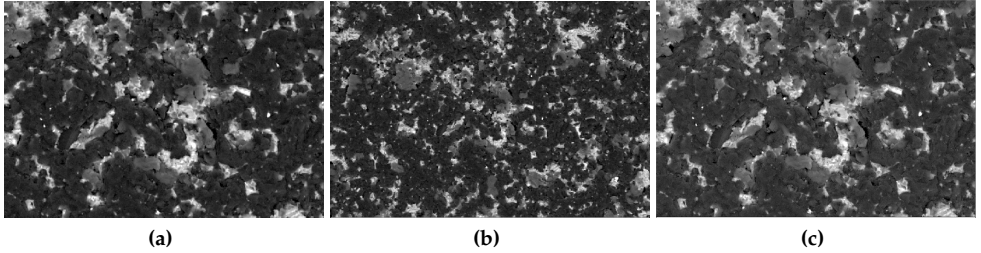


Figure 13: PCD grade 820 unpolished specimen surface microscopic images, a) SEM image before experiment at $10\mu\text{m}$, b) SEM image before experiment at $20\mu\text{m}$, c) EDX image of grade 820

crostructure remains consistent in polished and unpolished conditions, with only minor differences arising from the rougher grinding of unpolished samples.

2.3 Results

This section discusses the Tribotest results for the PCD samples under different loading conditions. The test was run for approximately 100 seconds at a frequency of 5Hz, with no lubrication between the contact surfaces, covering a sliding distance of approximately 3.5mm.

Figs. 14 and 15 illustrate the results for PCD grade 600 and grade 820 at 350N of polished and unpolished surfaces in Figs. 14 (a) and (c), the friction force is low, with a lower friction coefficient due to the polished surface. On the other hand, Fig. 14 (b) and (d) show very high friction force with a high friction coefficient because of the unpolished surface. Moreover, in both the unpolished surface of grade 600 and grade 820, grade 820 shows a high friction force compared to grade 600. Fig. 15 shows the normal forces in which there is no difference for both grades for polished and unpolished surfaces. The normal force in the complete test is not constant w.r.t to time, showing a sinusoidal pattern because of some vibration in the test rig. The results suggest that surface finish plays a crucial role in the tribological behaviour of PCD samples under the specified loading conditions. The higher surface roughness of unpolished samples leads to increased friction forces, highlighting the importance of surface treatment in reducing friction and wear.

Figs. 16 - 19 illustrate the results with different loadings, i.e., 550N and 1300N, showing the same trend of the figure for 350N with the same explanation for friction

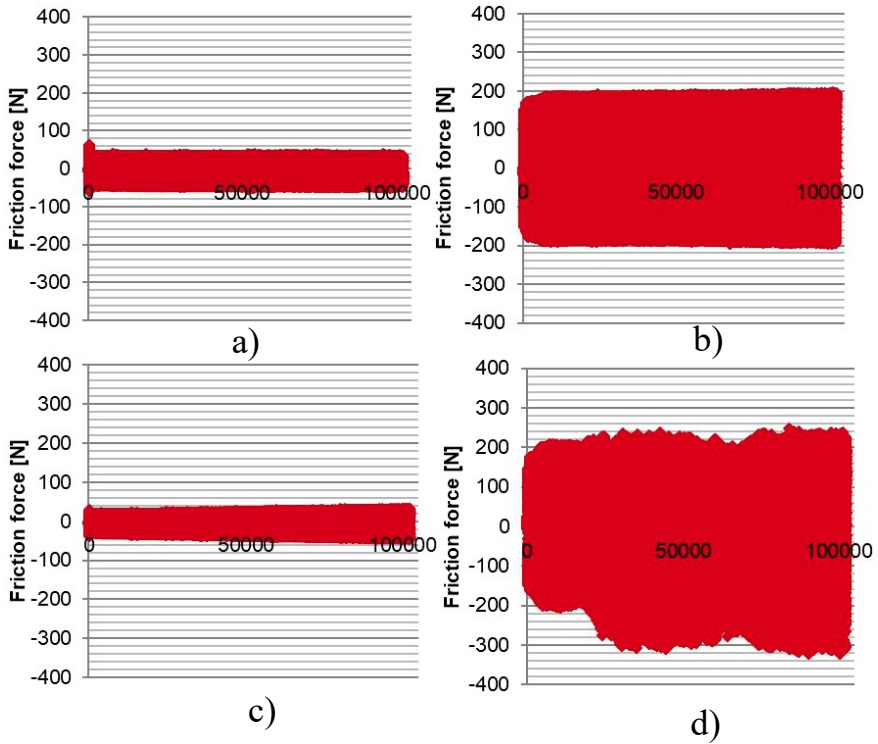


Figure 14: Time (in microseconds) vs Friction Forces during the Tribotest at 350N, a) grade 600 polished, b) grade 600 unpolished, c) grade 820 polished and d) grade 820 unpolished

and normal forces.

The results show that friction and normal forces change with varying loads; the applied and surface conditions affect friction forces, including whether the surfaces are unpolished or polished. This implies that surfaces with greater roughness and higher normal force experience increased friction forces, leading to a higher coefficient of friction and elevated surface wear. The variation in normal forces during the test due to vibration is also observed. The experimental data further indicates that the relation between frictional and applied normal forces is non-linear, suggesting complex interactions between the surfaces in contact. These outcomes align with prior research on how surface roughness and normal force impact frictional behaviour.

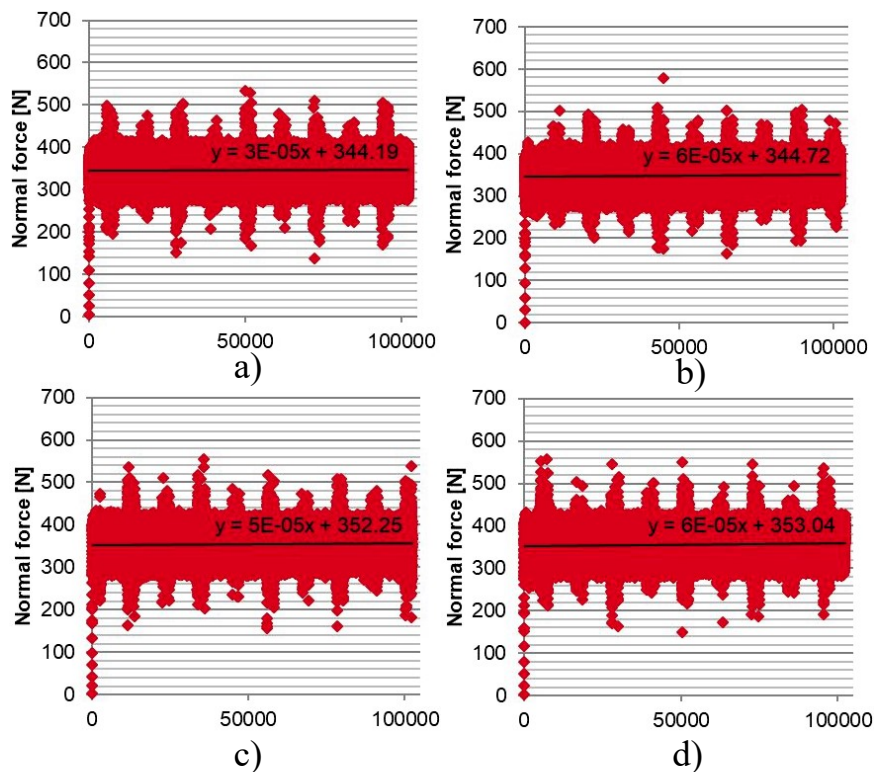


Figure 15: Time (in microseconds) vs Normal Forces during the tribotest at 350N, a) grade 600 polished, b) grade 600 unpolished, c) grade 820 polished and d) grade 820 unpolished

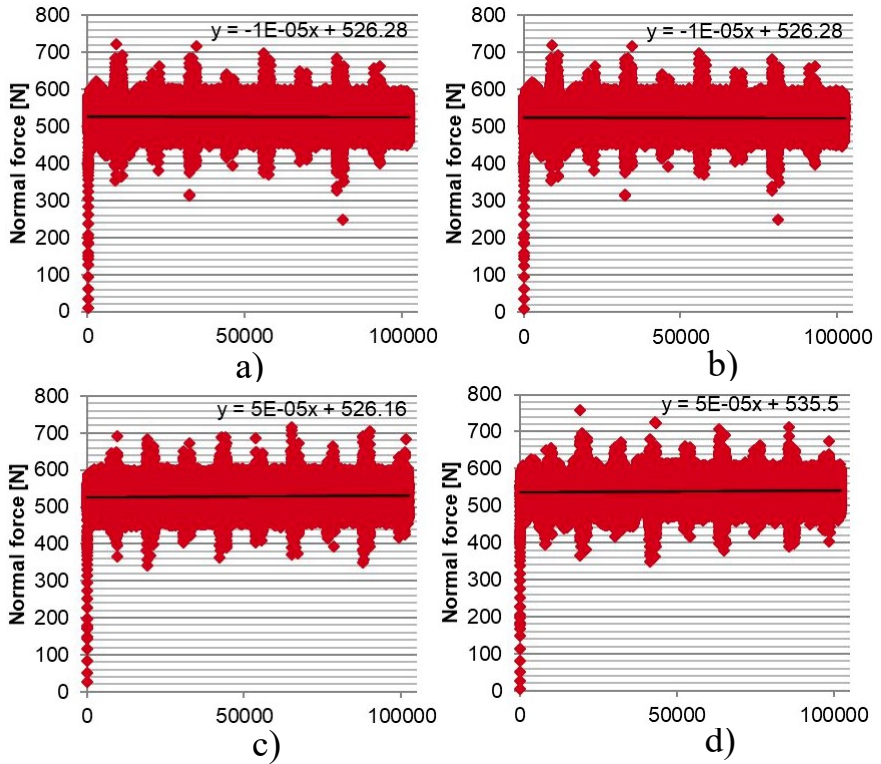


Figure 16: Time (in microseconds) vs Normal Forces during the Tribotest at 550N, a) grade 600 polished, b) grade 600 unpolished, c) grade 820 polished and d) grade 820 unpolished

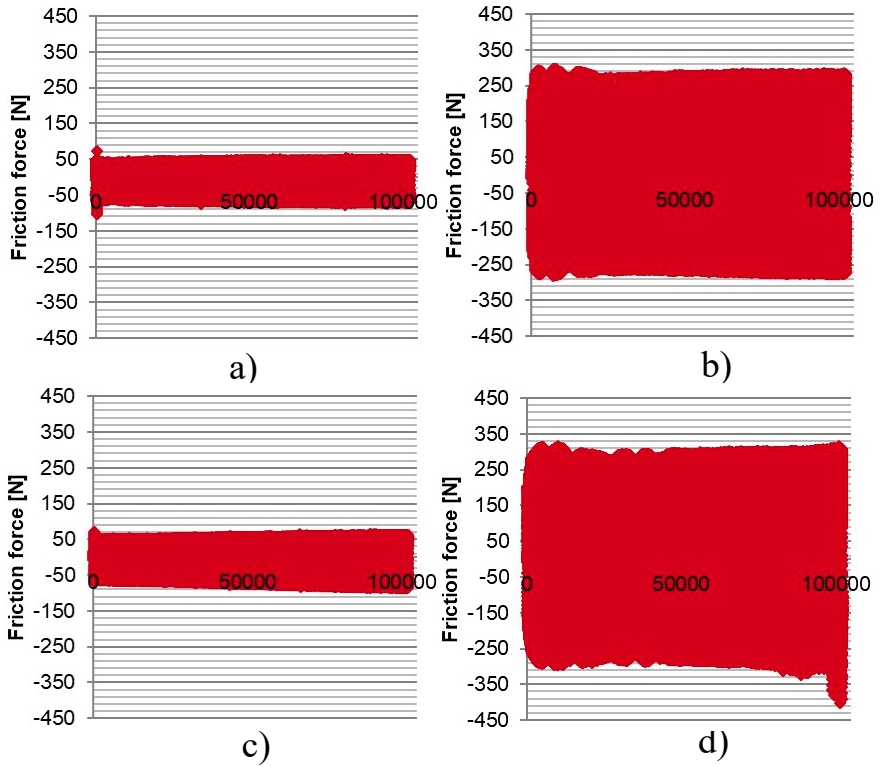


Figure 17: Time (in microseconds) vs Friction Forces during the Tribotest at 550N, a) grade 600 polished, b) grade 600 unpolished, c) grade 820 polished and d) grade 820 unpolished

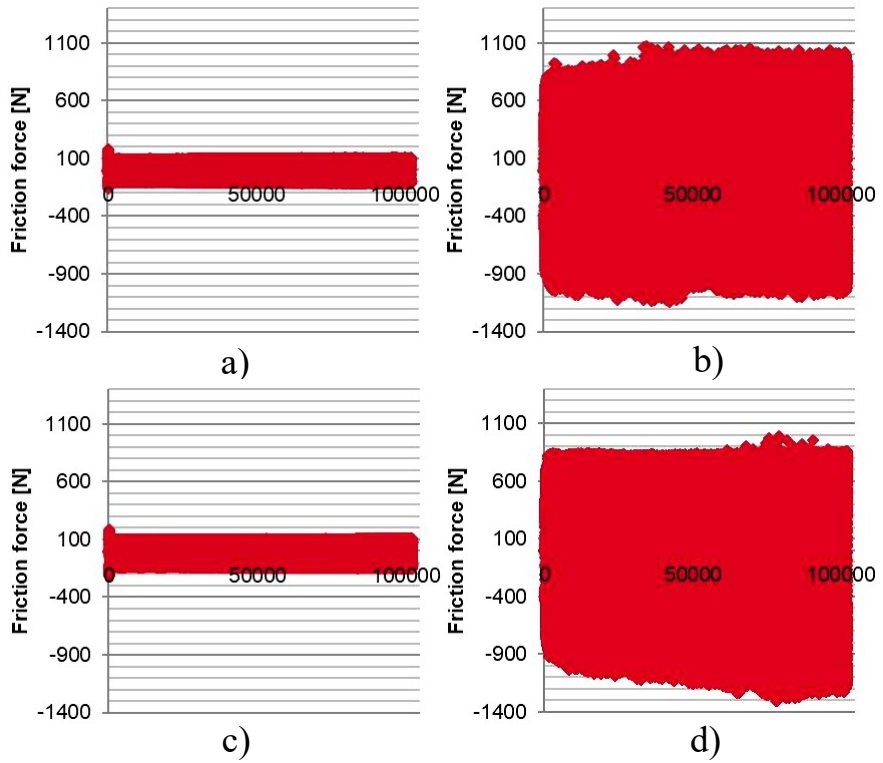


Figure 18: Time (in microseconds) vs Friction Forces during the Tribotest at 1300N, a) grade 600 polished, b) grade 600 unpolished, c) grade 820 polished and d) grade 820 unpolished

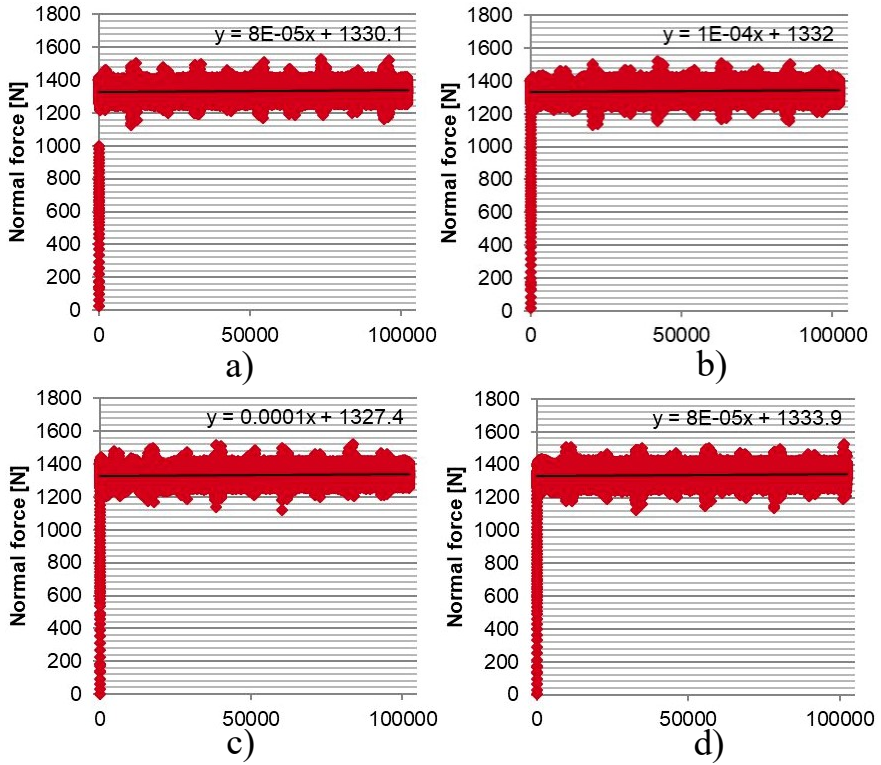


Figure 19: Time (in microseconds) vs Normal Forces during the Tribotest at 1300N, a) grade 600 polished, b) grade 600 unpolished, c) grade 820 polished and d) grade 820 unpolished

The Tribotest was conducted on grade 600 and grade 820 PCD samples, and different wear tracks were developed on the specimens. An optical microscope of stereo microscope type was employed to analyze the worn surfaces post-test. The images show the correlation between the wear tracks and the surface conditions, including the unpolished and polished surfaces, with the applied load. In Figs. 20 and 21, the specimens considered were polished and unpolished of grade 600 at different loads. It is seen from the pictures that because of the difference in surface profile, the wear track developed in the red colour line is also different in polished and unpolished. Moreover, different loads were considered in the test, which shows that different loads do not make much difference in the unpolished specimens. In contrast, the polished specimen showed some difference when the load was 1300N. Additionally, for the specimen of grade 820, the wear track tells us the same explanation as for grade 600, except that in the grade 820 polished specimen, the wear track was developed in the vertical direction in all the loadings, which shows that grade 820 is less wear resistance in machining operations. Furthermore, The grade 600 PCD sample's wear tracks show a different pattern than the grade 820 PCD sample, indicating variations in wear behaviour between the two grades. The analysis of these wear tracks provides valuable insights into the wear mechanisms of PCD materials under different loading conditions. The wear track analysis also revealed differences in wear mechanisms between polished and unpolished surfaces within each grade of PCD. The surface imperfections and roughness of the unpolished samples led to more severe wear than on the polished samples. This suggests that surface finish plays a crucial role in determining the wear resistance of PCD materials. The results of this study highlight the importance of understanding the relationship between surface conditions, applied loads, and wear behaviour in PCD materials.

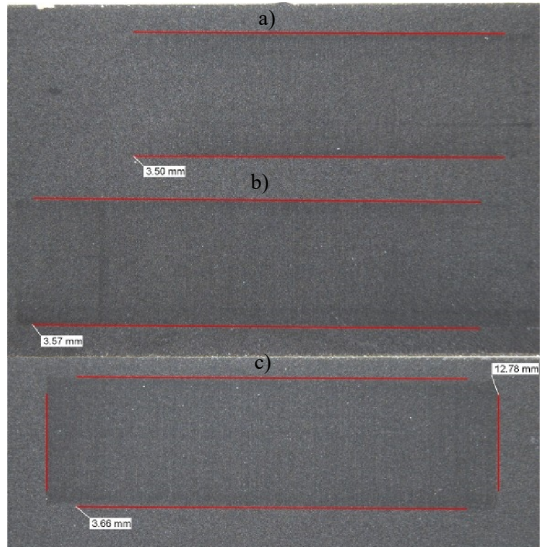


Figure 20: PCD 600-polished wear track, a) at 350N ,b) at 550N and c) at 1300N

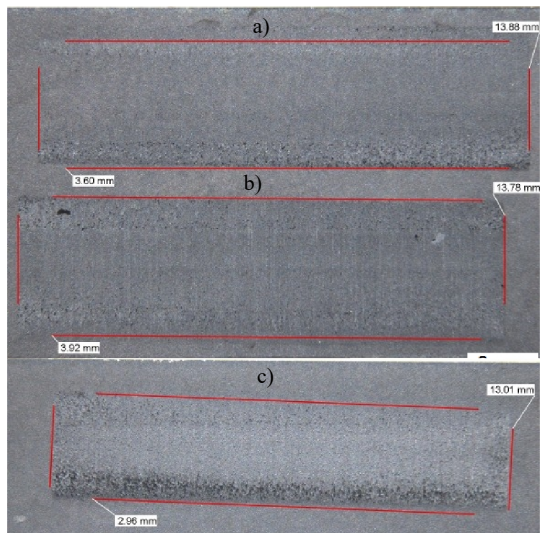


Figure 21: PCD 600-unpolished wear track, a) at 350N ,b) at 550N and c) at 1300N

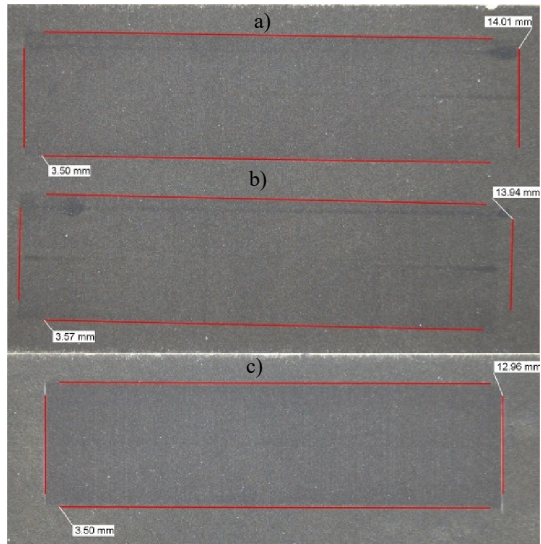


Figure 22: PCD 820-polished wear track, a) at 350N ,b) at 550N and c) at 1300N

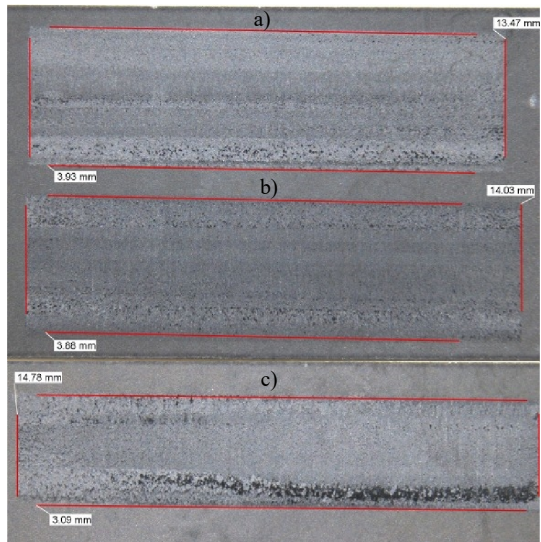


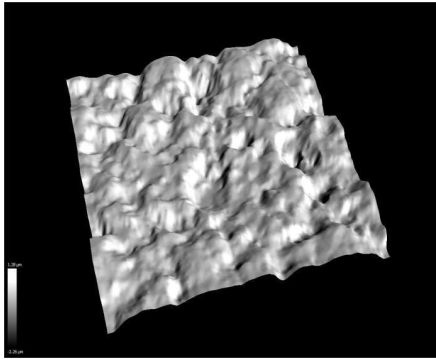
Figure 23: PCD 820-unpolished wear track, a) at 350N ,b) at 550N and c) at 1300N

2.4 Profilometric Analysis

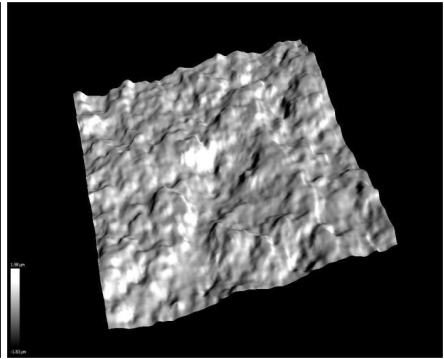
The samples' surface properties may differ from the unused ones, which requires a comprehensive evaluation. Surface data were collected using a non-contact LEICA DCM3D confocal profilometer at the MUSAM-Lab, IMT School of Advanced Studies Lucca, to establish a statistically representative surface for each sample type. A statistically representative surface should have sufficient troughs and peaks to adequately capture the overall surface's statistical properties. Using the profilometer's tool, the scanned area was expanded by stitching smaller regions together.

Fig. 24 presents the profile images of unused polished surface samples of grade 820 and grade 600 before testing. The images vividly depict the surface finish. The unpolished grade 820 sample displays a coarse and irregular surface, unlike the polished grade 820 sample, which shows a much smoother and more uniform finish. Similarly, the unpolished grade 600 sample demonstrates a rough surface, whereas the polished grade 600 sample has a markedly enhanced surface finish. These images visually demonstrate the effect of polishing on the surface quality of the PCD samples.

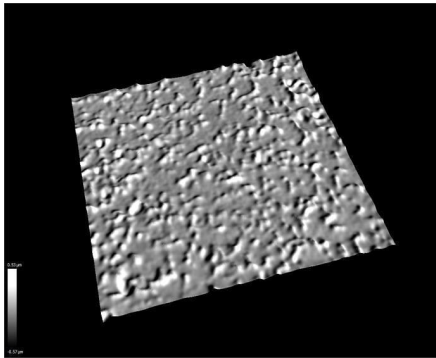
Figs. 25-26 present profile images of unpolished and polished surfaces of grade 820 and grade 600 after testing with different applied loads. The photos exhibit notable variations in surface texture and defects emerging on the surface post-test between the two PCD sample grades.



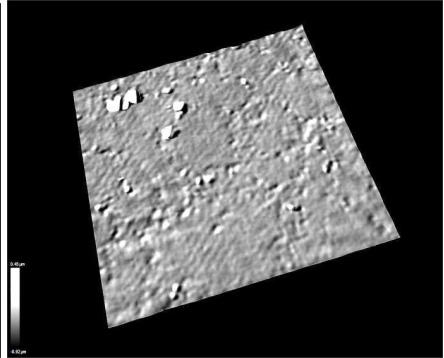
(a) Grade 820 unpolished



(b) Grade 600 unpolished

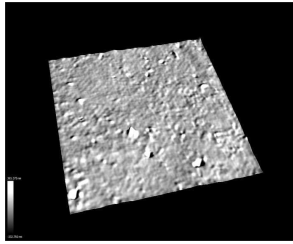


(c) Grade 820 polished

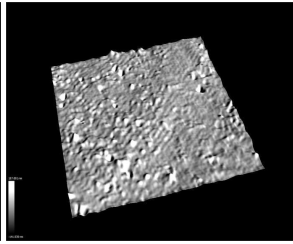


(d) Grade 600 polished

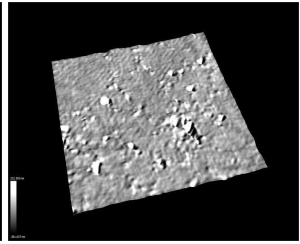
Figure 24: Confocal profilometer images of unused PCD samples of grade 600 and 820, polished and unpolished.



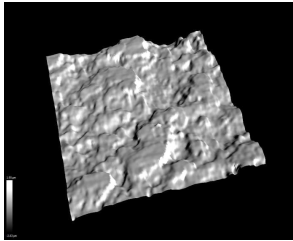
(a) Polished at 350N



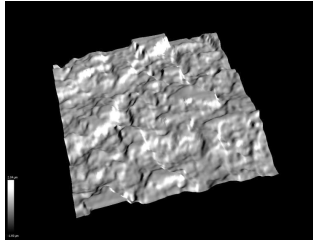
(b) Polished at 550N



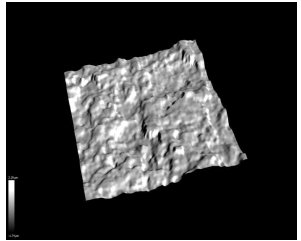
(c) Polished at 1300N



(d) Unpolished at 350N

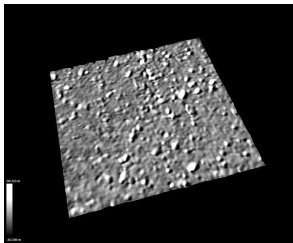


(e) Unpolished at 550N

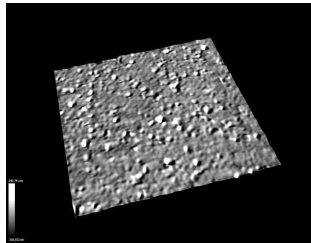


(f) Unpolished at 1300N

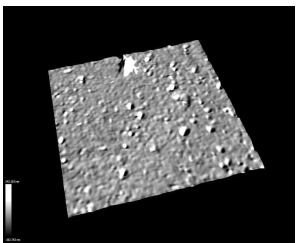
Figure 25: Confocal profilometer images of PCD of grade 600 after the test.



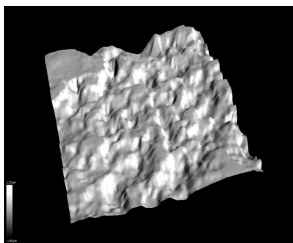
(a) Polished at 350N



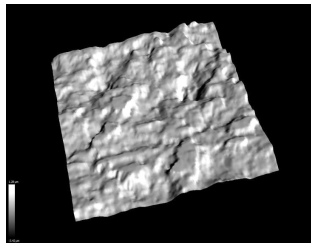
(b) Polished at 550N



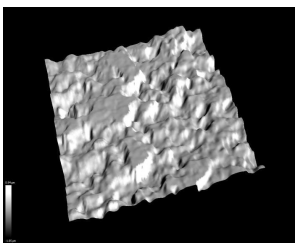
(c) Polished at 1300N



(d) Unpolished at 350N



(e) Unpolished at 550N



(f) Unpolished at 1300N

Figure 26: Confocal profilometer images of PCD of grade 820 after the test.

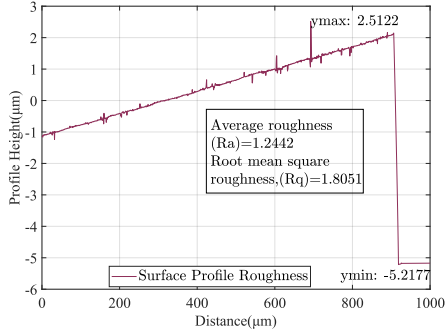
2.4.1 Surface Roughness Profiles

Surface roughness is the irregularity of the surface profile caused by manufacturing processes. These surface defects can result from unwanted vibrations, chatter, reflection, and straining of the materials. Because of the irregularities or defects on the surface, the surface is not considered a smooth surface.

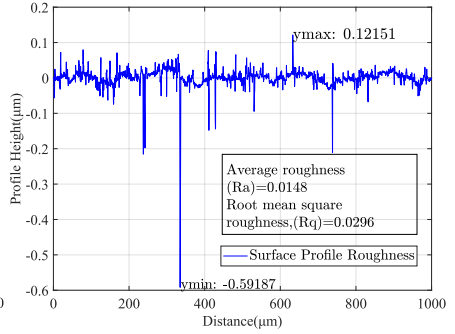
Generally, it is observed that the coefficient of friction of a rougher surface is usually higher than that of smooth surfaces. Furthermore, rough surfaces are also associated with cracks and corrosion nucleation sites, and rough surfaces may have a greater tendency to promote adhesion, which are other factors that affect surface roughness.

It was concluded from the experiment that two sample grades would be considered: polished and unpolished. In Fig. 27 and 28, we show the polished and unpolished surface of grade 600 roughness at various loads, respectively. Figs. 27 and 28 both (a) are the results for unused samples of grade 600, and the remaining results pertain to the worn section of the specimen's surface post-experiment grade 600 at different loads, i.e. 350N, 550N and 1300N.

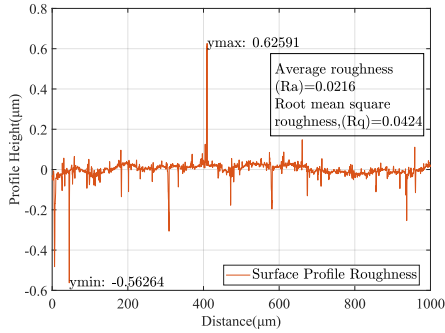
The analysis represents the average roughness, R_a , Root mean square, R_q , and the maximum height(peak) and maximum height(valley) of the roughness of the profile. Both R_a and R_q are critical and stable parameters that are not significantly affected by scratches, contamination, and measurement uncertainty. However, we know, in theory, that the difference in the roughness of smooth and rough surfaces depends on working conditions; therefore, from the results, it is seen that a polished specimen is reflected as a smooth surface as compared to a rough, unpolished specimen by showing lesser profile roughness height of the peak and valley. In contrast, on the other hand, unpolished specimen Fig.28 shows a much higher profile roughness height of the peak and valley. A similar explanation is for Fig.30 and 30.



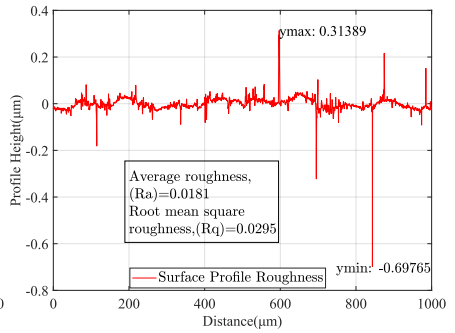
(a) Unused sample



(b) Tested at 350N

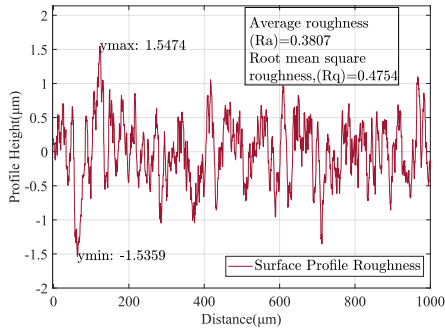


(c) Tested at 550N

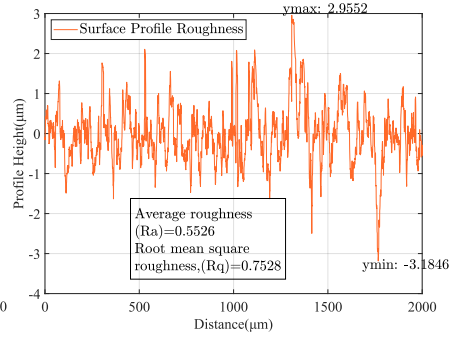


(d) Tested at 1300N

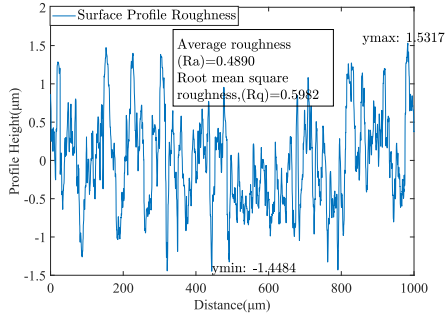
Figure 27: Surface roughness profile of a polished sample of grade 600 before experiment in (a) and after the test at different loads in (b)-(d).



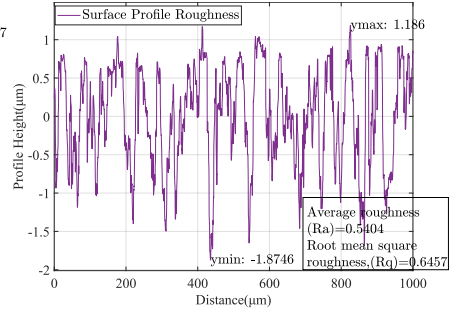
(a) Unused sample



(b) Tested at 350N

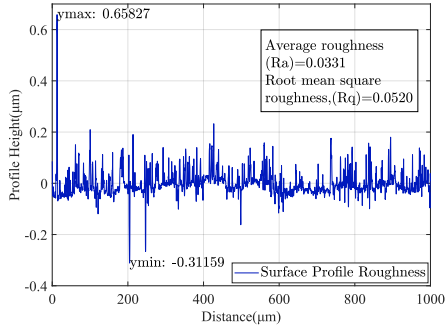


(c) Tested at 550N

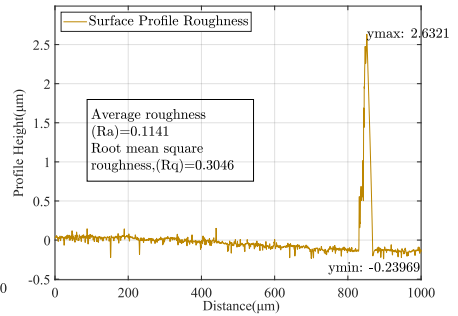


(d) Tested at 1300N

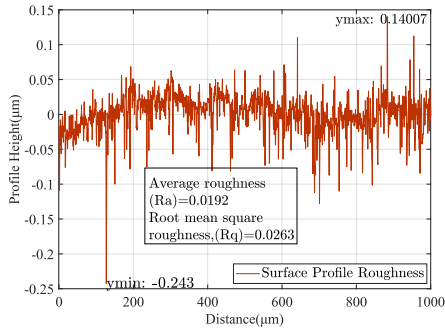
Figure 28: Surface roughness profile of an unpolished sample of grade 600 before experiment in (a) and after the test at different loads in (b)-(d).



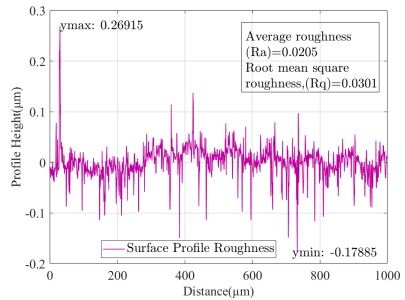
(a) Unused sample



(b) Tested at 350N

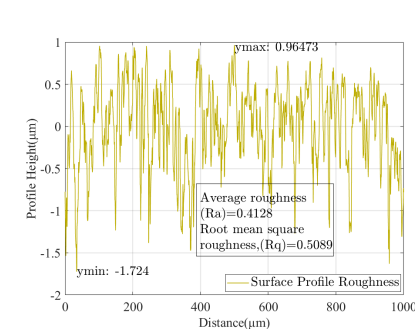


(c) Tested at 550N

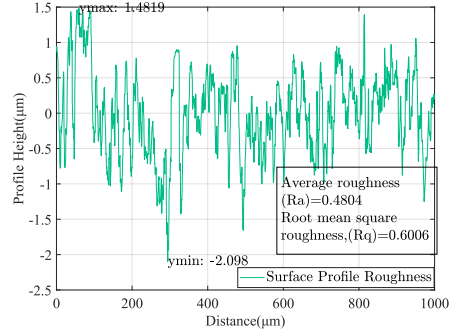


(d) Tested at 1300N

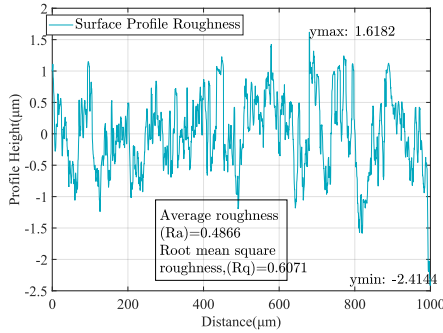
Figure 29: Surface roughness profile of a polished sample of grade 820 before experiment in (a) and after the test at different loads in (b)-(d).



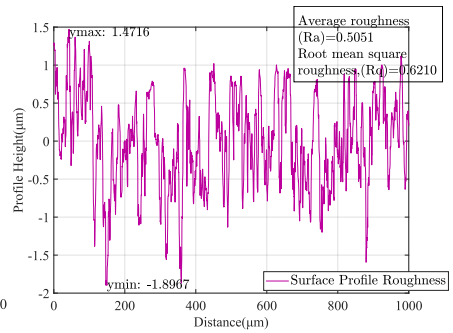
(a) Unused sample



(b) Tested at 350N



(c) Tested at 550N



(d) Tested at 1300N

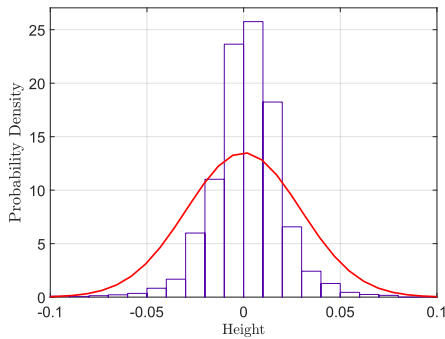
Figure 30: Surface roughness profile of an unpolished sample of grade 820 before experiment in (a) and after the test at different loads in (b)-(d).

2.4.2 Probability Density for the rough surface

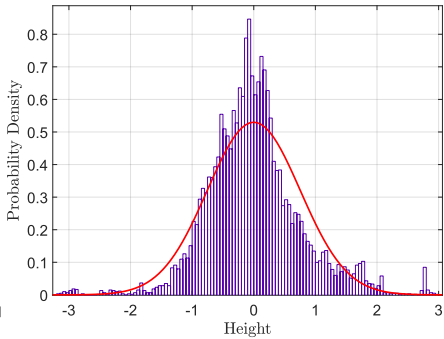
The probability function indicates the likelihood that a roughness profile has a specific height at a given position, which is mathematically referred to as a moment. The first moment corresponds to the arithmetic average, whereas the second moment relates to the variance or range of the roughness profile's height. The third moment, known as the skewness, represents the asymmetry of the amplitude distribution function. Positive skewness denotes material accumulation near the bottom of the profile, while negative skewness signifies accumulation near the top. The fourth moment, kurtosis, quantifies the sharpness of the amplitude distribution function. A flat amplitude distribution suggests numerous small, rounded peaks and valleys in the roughness profile. The total area under the probability density function must be equal to one, ensuring that the value of z at any x is between $+\infty$ and $-\infty$, or between $z_{\max}$ and $z_{\min}$. Data depicting random physical phenomena often follow a Gaussian or normal probability density function.

$$p(z) = \frac{1}{\sigma(2\pi)^{1/2}} \exp\left[-\frac{(z - m)^2}{2\sigma^2}\right] \quad (2.1)$$

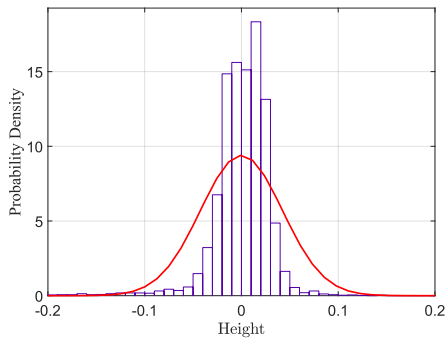
where μ is the standard deviation and m is the mean. A height distribution, or a histogram, is a statistical representation of an object's height in terms of a probabilistic function $p(z)$ when the object's height is considered random. [15, 16]. Figs. 31 to 32 illustrate the distribution of surface heights as a function of the probability density of polished and unpolished surfaces under different loads, i.e. 350N, 550N and 1300N, indicating that polished surfaces exhibit fewer data points under the probability density curve than unpolished surfaces at different load levels. Since the unpolished surface has greater roughness, the area under the curve is more significant for the unpolished surface, indicating more roughness height data. The Gaussian curves demonstrate different peak values and include an analysis of kurtosis, which measures the 'tailedness' of the probability distribution. The symmetric curves indicate zero skewness, meaning the data are evenly distributed around the mean (μ). Furthermore, based on the Empirical Rule, 68% of the surface height data falls within 1st standard deviation (σ) from the mean (μ), which is regarded as the average roughness height. At 2nd standard deviation (σ) from the mean (μ), 95% of the surface height data is encompassed, and at 3rd standard deviation (σ), this jumps to 99%. Additionally, the left side of the curve corresponds to lower mean (μ) values of surface roughness, while the right side corresponds to higher mean (μ) values.



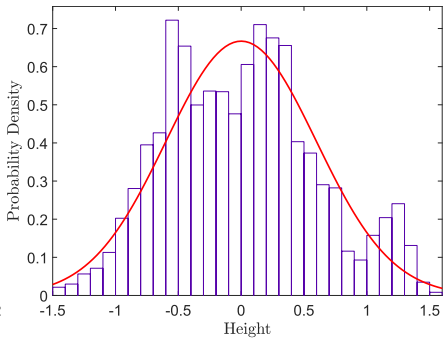
(a) Polished 600 grade sample at 350N



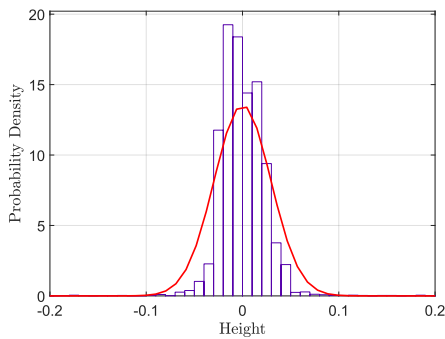
(b) Unpolished 600 grade sample at 350N



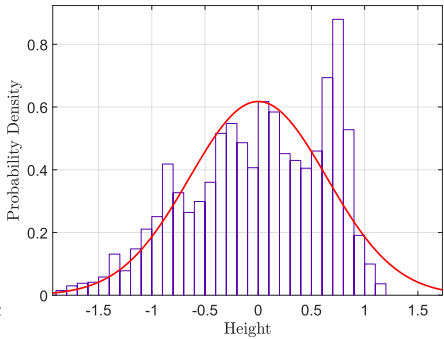
(c) Polished 600 grade sample at 550N



(d) Unpolished 600 grade sample at 550N

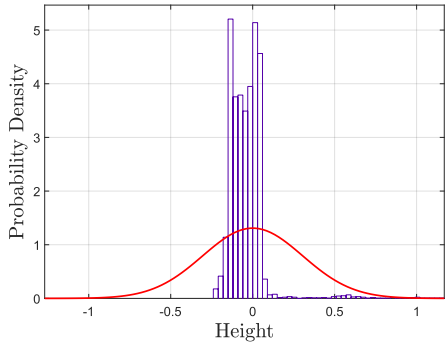


(e) Polished 600 grade sample at 1300N

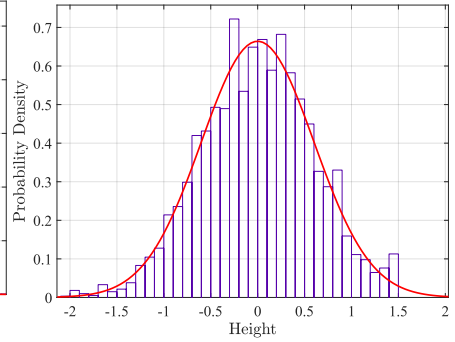


(f) Unpolished 600 grade sample at 1300N

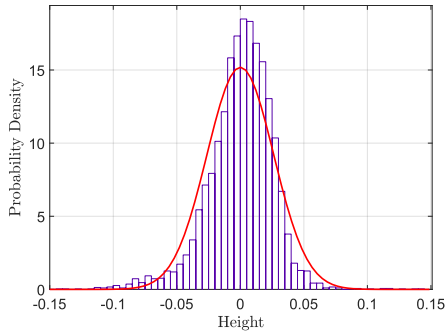
Figure 31: Probability density of the worn surface after experimenting with PCD samples of grade 600, polished and unpolished at different loads.



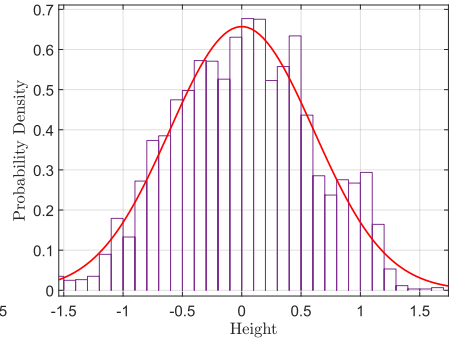
(a) Polished 820 grade sample at 350N



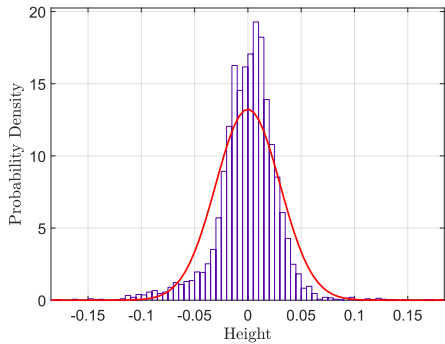
(b) Unpolished 820 grade sample at 350N



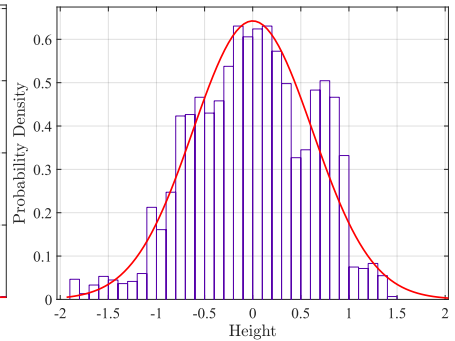
(c) Polished 820 grade sample at 550N



(d) Unpolished 820 grade sample at 550N



(e) Polished 820 grade sample at 0300N



(f) Unpolished 820 grade sample at 1300N

Figure 32: Probability density of the worn surface after experimenting with PCD sample of grade 820, polished and unpolished at different loads.

Chapter 3

Theoretical Model And Computational Aspects

3.1 Introduction

In this chapter, we first review the equilibrium equations related to the elastic material. Using energy considerations, the thermodynamic consistency of the equilibrium equation is discussed. Invoking the second law of thermodynamics, equilibrium equations are modified to accommodate wear resistance resulting from friction between two contact surfaces due to complex rough surfaces. These developments discuss a thermodynamically consistent wear model within the context of the equilibrium equations. A finite element method is proposed based on the embedded roughness via composite topography. The specific aspects regarding Anzats, discretization, composite topography, and wear laws are discussed in the sequel. Moreover, an extension to include the thermomechanical wear capable of computing wear rate due to friction between the surfaces considering the heat generated between the system is proposed using the embedded roughness method.

3.1.1 Equilibrium Equations

This section briefs on the fundamentals of continuous solid mechanics (CSM), which form the foundation of computational mechanics. Continuum mechanics describes the motion of a body under external forces. Consider an arbitrary body $\mathcal{B} \in \mathbb{R}^{n_{dim}}$ ($n_{dim} = 1, 2, 3$) in Euclidean space with its delimiting boundaries defined as $\partial\mathcal{B} \in \mathbb{R}^{n_{dim}-1}$.

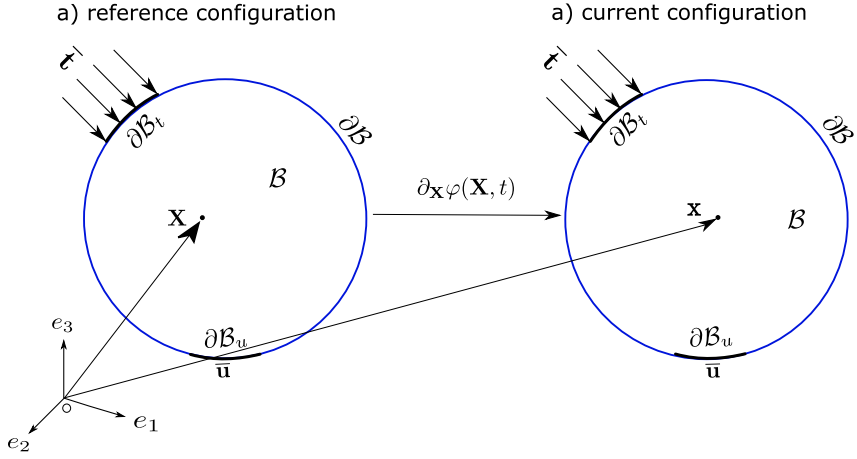


Figure 33: Finite Deformation of a body: reference and current configuration.

The continuum of the body $\mathcal{B}$ is defined by a position vector $\mathbf{X} = [x_1, x_2, x_3]$. The motion of the body from a deformed state characterized by deformation field $\mathbf{u}(\mathbf{X}, t) : \mathcal{B} \times [0, t] \rightarrow \mathbb{R}^{n_{dim}}$ such that the current position vector $\mathbf{x}$ of the material point takes the form:

$$\mathbf{x}(\mathbf{X}, t) = \mathbf{X} + \mathbf{u}(\mathbf{X}, t). \quad (3.1)$$

This forms the basis of the Lagrangian view of the system. In addition, t in the quasi-static sense is the pseudo-time, whose consideration can be considered physical under a dynamic setting.

Naturally, the symmetric part of the displacement gradient $\nabla^{sym} \mathbf{u}$ is defined as strain measure ε , i.e:

$$\varepsilon = \nabla^{sym} \mathbf{u} = \frac{1}{2} [\nabla \mathbf{u} + \nabla^T \mathbf{u}]. \quad (3.2)$$

Based on Cauchy's stress principle, a symmetric second-order tensor $\boldsymbol{\sigma}$ of stresses exists in the current configuration due to external force acting on $\mathcal{B}$. The stresses satisfy local balance of momentum at all points $\mathbf{X} \in \mathcal{B}$ i.e:

$$\text{div } \boldsymbol{\sigma} + \mathbf{f}_v = 0, \quad (3.3)$$

where $\text{div} [\cdot]$ is the divergence operator and $\mathbf{f}_v$ denotes the external forces. The stresses $\boldsymbol{\sigma}$ or the displacement $\mathbf{u}$ is assumed to be consequence of the prescribed

- (i) displacement $\mathbf{u} = \bar{\mathbf{u}}$ on $\partial \mathcal{B}_u$,
- (ii) traction $\bar{\mathbf{t}} = \boldsymbol{\sigma} \cdot \mathbf{n}(x, t)$ on $\partial \mathcal{B}_t$ for an outward normal $\mathbf{n}$,

such that $\partial\mathcal{B}=\partial\mathcal{B}_u \bar{\cup} \partial\mathcal{B}_t$ and $\partial\mathcal{B}_u \cap \partial\mathcal{B}_t=\emptyset$ as in Fig 33.

The stress state of any system can be represented only by its strain state as $\boldsymbol{\sigma} = \boldsymbol{\sigma}(\boldsymbol{\varepsilon})$. In the elastic regime, state $\boldsymbol{\sigma}$ is independent of the path taken. Mathematically, such path independence is guaranteed if and only if rate potential function $\mathcal{W}(\boldsymbol{\varepsilon})$ concerning $\boldsymbol{\varepsilon}$ exists i.e.

$$\boldsymbol{\sigma} := \frac{\partial\mathcal{W}(\boldsymbol{\varepsilon})}{\partial\boldsymbol{\varepsilon}}. \quad (3.4)$$

On the other hand, if the deformation is path-independent, the corresponding material law is termed hyper-elastic. The consistent derivation of stress concerning strain yields modulus of elasticity or constitutive tensor or material tensor $\mathbb{C}$. This material tensor can also be seen as a liner mapping of the strain tensor into the stress tensor,

$$\mathbb{C} := \frac{\partial\boldsymbol{\sigma}(\boldsymbol{\varepsilon})}{\partial\boldsymbol{\varepsilon}} = \frac{\mathcal{W}(\boldsymbol{\varepsilon})}{\partial\boldsymbol{\varepsilon} \otimes \partial\boldsymbol{\varepsilon}}. \quad (3.5)$$

Since stress and strain are second-order tensors, the material tensor $\mathbb{C}$ is a fourth-order tensor. Consequently, stresses can be computed as a direct result of strain via $\mathbb{C}$ as

$$\boldsymbol{\sigma} = \mathbb{C} : \boldsymbol{\varepsilon}. \quad (3.6)$$

If the material tensor $\mathbb{C}$ is strain independent, meaning that a linear relation exists between stress $\boldsymbol{\sigma}$ and strain $\boldsymbol{\varepsilon}$, we refer to the Eq. (3.6) as linear constitutive law. In the three-dimensional setting and using vectoring notations for stress and strain, Eq. (3.6) can be expanded as

$$\begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{12} \\ \sigma_{23} \\ \sigma_{13} \end{bmatrix} = \begin{bmatrix} \mathbb{C}_{1111} & \mathbb{C}_{1122} & \mathbb{C}_{1133} & \mathbb{C}_{1112} & \mathbb{C}_{1123} & \mathbb{C}_{1113} \\ \mathbb{C}_{2211} & \mathbb{C}_{2222} & \mathbb{C}_{2233} & \mathbb{C}_{2212} & \mathbb{C}_{2223} & \mathbb{C}_{2213} \\ \mathbb{C}_{3311} & \mathbb{C}_{3322} & \mathbb{C}_{3333} & \mathbb{C}_{3312} & \mathbb{C}_{3323} & \mathbb{C}_{3313} \\ \mathbb{C}_{1211} & \mathbb{C}_{1222} & \mathbb{C}_{1233} & \mathbb{C}_{1212} & \mathbb{C}_{1223} & \mathbb{C}_{1213} \\ \mathbb{C}_{2311} & \mathbb{C}_{2322} & \mathbb{C}_{2333} & \mathbb{C}_{2312} & \mathbb{C}_{2323} & \mathbb{C}_{2313} \\ \mathbb{C}_{1311} & \mathbb{C}_{1322} & \mathbb{C}_{1333} & \mathbb{C}_{1312} & \mathbb{C}_{1323} & \mathbb{C}_{1313} \end{bmatrix} \begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ 2\varepsilon_{12} \\ 2\varepsilon_{23} \\ 2\varepsilon_{13} \end{bmatrix} \quad (3.7)$$

All the other materials, including anisotropy plasticity and non-linearity, can be introduced into the system via the material model in Eq. (3.6).

3.1.2 Weak Forms

The local behaviour at each point $\boldsymbol{x} \in \mathcal{B}$ can be described using the balance equilibrium equation in Eq. (3.3) along with the boundary values. This is referred to as the

governing equation in strong forms; writing the Eq. (3.3) in terms of displacement, we have

$$\text{div}(\mathbb{C} : \nabla^{sym} \mathbf{u}) + \mathbf{f}_v = 0, \forall \mathbf{x} \in \mathcal{B}. \quad (3.8)$$

For us to solve for the displacement field in Eq. (3.8), the problem must be solved at each material point. Moreover, it is expected to find a Laplacian of the field. Mathematically, the least possible space in which Eq. (3.8) holds translates to

$$\mathbf{u} \in \mathcal{B}^u := \{\mathbf{u} \in \mathbf{H}^2(\mathcal{B}) : \mathbf{D}^2 \mathbf{u} \in \mathbf{L}^2(\mathcal{B})\}. \quad (3.9)$$

Note that $\mathbf{u} \in \mathcal{B}^u$ is well posed because $\mathbf{u}$ has to be at least two times differentiable, at least in the sense of approximation of the equilibrium equations. Moreover, for every material point $\mathbf{X} \in \mathcal{B}$, satisfying Eq. (3.8) is arduous. Hence, we resort to weak form, leading to a Ritz/Galerkin type approximation so that functional space can be constructed via finite element methods, solving the issue of well-pseudo and due to the innate nature of weak forms, the state's conditions in Eq. (3.8) must be satisfied only in an average sense.

Weak forms, referred to as integral forms, are often a direct consequence of virtual work or variational formulation. It is important to note that a weak form having enough regularity of $\mathbf{u}$ leads to a strong form.

Integral forms of energy are used widely. This facilitates a clear understanding of the physics involved in the sense of energies, and it is easy to convert into weak form, eventually leading to the Galerkin/Ritz method. In this regard, the balance in the Eq. (3.8) can be written as a conservation of linear momentum, i.e.:

$$\Pi(\mathbf{u}) = \Pi_{int}(\mathbf{u}) + \Pi_{ext}(\mathbf{u}), \quad (3.10)$$

where the total energy $\Pi(\mathbf{u})$ is combination of external energy applied to system $\Pi_{ext}(\mathbf{u})$ denoted as:

$$\Pi_{ext}(\mathbf{u}) := - \int_{\mathcal{B}} \mathbf{f}_v \cdot \mathbf{u} dV - \int_{\mathcal{B}_{\sqcup}} \bar{\mathbf{t}} \cdot \mathbf{u} dS. \quad (3.11)$$

where $\mathbf{f}_v : \mathcal{B} \rightarrow \mathbb{R}^{n_{dim}}$ is the distributed body force. As a response to the externally applied load, the body under consideration undergoes deformation, creating an internal resistance or elastic energy the body denoted as $\Pi_{int}(\mathbf{u})$ as,

$$\Pi_{int}(\mathbf{u}) = \int_{\mathcal{B}} \mathcal{W}(\varepsilon(\mathbf{u})) dV = \int_{\mathcal{B}} \boldsymbol{\sigma}(\varepsilon(\mathbf{u})) : \varepsilon(\mathbf{u}) dV. \quad (3.12)$$

Notice that, to solve Eq. (3.10) using the Galerkin method, the regularity restriction required for displacement field $\mathbf{u}$ is compromised to $\mathbf{u} \in \mathcal{U}^u$ with $\mathcal{U}^u := \{\mathbf{u} \in H^1(\mathcal{B}) : \nabla \mathbf{u} \in L^2(\mathcal{B}); \mathbf{u} = \bar{\mathbf{u}} \text{ on } \partial\mathcal{B}\mathbf{u}\}$.

The solution of Eq. (3.10) is then obtained as a minimization problem i.e. find $\mathbf{u}^* \in \mathcal{U}^u$ such that

$$\mathbf{u}^* = \text{Argmin}_{\mathcal{U}^u} \lim\{\Pi(\mathbf{u})\}. \quad (3.13)$$

As a natural consequence of the minimization problem, the first variation of $\Pi(\mathbf{u})$ satisfies linear momentum, i.e.

$$\delta\Pi(\mathbf{u}) = \delta\Pi_{int}(\mathbf{u}) + \delta\Pi_{ext}(\mathbf{u}) = 0, \quad (3.14)$$

with δf defined in the sense of Gateaux derivatives as

$$\delta f(\mathbf{u}) = \lim_{e \rightarrow 0} \frac{f(\mathbf{u}) + f(\mathbf{u} + e\delta\mathbf{u})}{e}. \quad (3.15)$$

For a small perturbation $\delta\mathbf{u} \in \mathcal{V}^u$ (often referred as test function) with $\mathcal{V}^u = \{\delta\mathbf{u} \in H^1(\mathcal{B}) : \delta\mathbf{u} = 0 \text{ on } \partial\mathcal{B}\mathbf{u}\}$, for some direction e .

In this context, Eq. (3.14) takes the form:

$$\begin{aligned} \delta\Pi_{int}(\mathbf{u}, \delta\mathbf{u}) &= \left\{ \int_{\mathcal{B}} \boldsymbol{\sigma}(\boldsymbol{\varepsilon}(\mathbf{u} + e\delta\mathbf{u})) : \boldsymbol{\varepsilon}(\mathbf{u} + e\delta\mathbf{u}) dV \right\} \Big|_{e=0} \\ &= \int_{\mathcal{B}} \boldsymbol{\sigma}(\boldsymbol{\varepsilon}(\mathbf{u})) : \boldsymbol{\varepsilon}(\delta\mathbf{u}) dV, \end{aligned} \quad (3.16)$$

and

$$\begin{aligned} \delta\Pi_{int}(\mathbf{u}, \delta\mathbf{u}) &= - \left\{ \int_{\mathcal{B}} (\mathbf{u} + e\delta\mathbf{u}) \cdot \mathbf{f}_v dV + \int_{\partial\mathcal{B}} (\mathbf{u} + e\delta\mathbf{u}) \cdot \bar{\mathbf{t}} \partial dV \right\} \Big|_{e=0} \\ &= - \int_{\mathcal{B}} \delta\mathbf{u} \cdot \mathbf{f}_v dV - \int_{\partial\mathcal{B}} \delta\mathbf{u} \cdot \bar{\mathbf{t}} \partial dV \end{aligned} \quad (3.17)$$

leading to:

$$\int_{\mathcal{B}} \boldsymbol{\sigma}(\boldsymbol{\varepsilon}(\mathbf{u})) : \boldsymbol{\varepsilon}(\delta\mathbf{u}) dV - \int_{\mathcal{B}} \delta\mathbf{u} \cdot \mathbf{f}_v dV - \int_{\partial\mathcal{B}} \delta\mathbf{u} \cdot \bar{\mathbf{t}} \partial dV \quad (3.18)$$

For all $\mathbf{u} \in \mathbf{u}^u$ and $\delta\mathbf{u} \in \mathbf{V}^u$. It is also easy to see that, integration by part of the above equation and assuming $\mathbf{u} \in H^2(\mathcal{B})$, we have:

$$\delta\mathbf{u}\{\text{div}\boldsymbol{\sigma} + \mathbf{f}_v\} = 0 \quad \text{on } \mathcal{B} \quad (3.19a)$$

$$\mathbf{t} = \boldsymbol{\sigma} \cdot \mathbf{n} \quad \text{on } \partial\mathcal{B}\mathbf{t} \quad (3.19b)$$

Now, it is easy to see that for all $\delta u \geq 0$ on $\mathcal{B}$, Eq. (3.19) reduces to Eq. (3.8) recovering governing equations in strong form. This is often called the system's first-order or thermodynamics stability condition.

In the following sections, we shall discuss the total energy of the system in Eq. (3.10) is modified to accommodate wear and eventually thermal effects by using a consistent choice of the constitutive law as in Eq. (3.6), the material behaviour is controlled. The weak forms of the variational formulation are then invoked to obtain Galerkin approximation, especially the finite-element method, which is discussed in the sequel.

3.1.3 Introduction

Every material in contact wears out over a period of time. Wear occurs when two or more materials are in contact due to sliding between the surfaces. Consequently, the material properties, such as toughness, are reduced, leading to a catastrophic failure. Under the influence of fatigue loads, wear seriously threatens engineering design. Nevertheless, predicting and controlling the wear of two rubbing surfaces is essential.

Contact regions commonly occur in mechanical devices and mechanisms, tools, and workpieces in the machining process. Mechanical loads and heat motion are transmitted through the contact surfaces, whereas friction and wear accompany sliding contact. In machine design, wear is considered an equally important reason for damage. Generally, before the advent of computational tools, the study of wear was restricted to environmental studies and empirical relationships. In contrast, new mathematical models nowadays predict wear numerically as precisely as possible. Due to the complex nature of wear, the efficiency and reliability of computational methods are still in their infancy and are ever-increasing as technology advances.

Literature regarding the numerical approximations of the wear is abundant. Early numerical analyses of worn-out solids were given by Hugnell et al. [17], Stromberg [18, 19], Szefer [20], Christensen et al. [21], Agelet de Saracibar and Chiumenti [22], Franklin et al. [23], Ko et al. [24], Shillor et al. [25], McColl et al. [26], Telliskivi [27], Kim et al [28]. In Particular, Szefer [20] and Stromberg [18, 19] looked at the evolution of wear gaps in fretting problems using the finite element method. The numerical study of pitting wear shapes by Glodez et al. [29, 30] was examined under various operating conditions using fracture mechanics techniques.

Several authors such as Suh [31], Rosenfield [32], Sin and Suh [33], Bogdaski et al. [34], and Dubourg et al. [35] have calculated surface or near-surface fatigue crack propagation due to contact stresses. Goryacheva [36] and Podra and Anderson [37] have proposed analytical approaches to wear. The mechanism of wear particle production has been simulated by Aghababaei et. al. [38] using molecular dynamics, extending the model to the multi-asperity case in Frérot et. al. [39] and to the adhesive wear process of rough surfaces in sliding contact in [40]. See [41] for an in-depth review of the wear.

Experimental investigation shows that, for the surfaces under contact, the roughness of the profiles plays a crucial role. Moreover, surfaces involved in most engineering applications show that roughness can range from a nano-scale to a milli-scale. Consequently, a proper surface geometry description can significantly improve the wear prediction, as the wear is related to the contact area. Many contact models have been developed to predict contact geometry. Prominent among them are Greenwood and Willianson's model [42], Mikic's elastic model [43], and Cooper, mikic, and Yovanovich's plastic model [44]. A detailed description of the input parameters for an isotropic and anisotropic cases for the GW model can be seen in [45].

Greenwood and Willianson's model [42] considers the contact between a rough surface and a flat, rigid surface. Consequently, the contact stemming from such an assumption leads to a rough surface in contact with an ideal plane. See [46] for more details. The deformations are considered elastic, and an equivalent composite property of the contacting bodies represents mechanical properties. The model has been revised by many authors, including but not limited to [47, 46, 48, 49]. More importantly, Chang et. al. [50] included a transition to a fully plastic case, whereas a closed-form solution was used for the GW model [51]. The effect of adhesion by considering Weibull distribution is reported in [52, 53].

Rough surfaces were characterized by a Gaussian distribution using peak linear density, mean absolute slope, and surface roughness in Cooper, Mikic, and Yovanovich models [44]. Hardness is considered in [44] in [54]. On the other hand, the Mikic model [43] assumes a similar geometrical model as in [44], whereas a statistical parameter representing area is proposed. Other rate dependence of contact predictions using fractal contact models can also be seen [55, 56, 57]. A detailed review and insights involving multi-scale contact predictions stemming from the classical stochastic models are presented in [58, 49].

Recently, numerical schemes based on the Boundary Element Method (BEM)

have been proposed to evaluate tangential contact problems with arbitrarily complex contact geometries, see [59, 60, 61]. BEM-based algorithm poses several limitations stemming from the material's linear elasticity assumptions, half space approximations, and homogeneity. Consequently, Finite Element Methods (FEM) are used to overcome the limitations imposed by BEM; see [62, 63, 64] for more details. Variational methods to contact based on the greenwood assumptions were introduced by Paggi et. al. [45]. This approach proposes a variational formulation to solve normal contact problems involving contact surfaces separated by a rough interface and shape. This approach considers the interface as typically flat and embeds an analytic expression of the roughness to correct the normal gaps in a cohesive zone-like interface. This allows any shape of the indenter or rough surfaces to be embedded in the contact profile. Consequently, this leads to a zero-thickness interface finite element with an embedded profile representing the joint roughness of the contact surfaces. This is referred to as the "MPJR (eMbedded Profile for Joint Roughness) interface finite element." See [45] for more details. As a consequence of the variational formulation, computational implementation can be easily achieved using implicit FE procedures. Moreover, the model can be easily extended to anisotropic solids. This modelling framework was extended to analyse fully coupled normal and tangential contact problems with complex surfaces by Bonari et. al. [65]. In anticipation of the thesis, the MPJR interface model is extended to accommodate wear. Moreover, a thermo-mechanical extension of the MPJR is provided in this thesis.

Several types of wear have been recognized to date; some of them are (a) abrasive, (b) adhesive, (c) fretting, (d) erosion, (e) oxidation, and (f) corrosion. Meanwhile, abrasive wear in the contact fatigue setting is crucial in the industry and this thesis.

Solid fundamentals and physics must be laid out to develop a computational model. In the process of wear, the material is removed from the surface of the contact solid and gradually worn out. The amount of material removed at any given point can be estimated using a wear profile. Wear depth defines the total removal of material over time, and wear rate corresponds to the rate at which material is removed. Qualitative information on wear can be obtained by visually inspecting the wear surface.

Furthermore, more detailed photographs can be used to inspect the wear in different instances. Equipment such as a scanning electron microscope and surface topography measurements in different cases can be used to estimate the wear pre-

cisely. By examining the history of such topographic measurements, wear rate can be estimated precisely.

From the numerical standpoint, the microscopic examination of the contact surfaces reveals the following details that lead to modelling techniques.

1. Contact surfaces have roughness associated with each other. Hence, not all parts of the surface are in contact. Hence, the contact surface strongly depends on the roughness profiles of the surface. A mathematical model needs to account for such roughness variations. Many authors have proposed different methods, for example, Greenwood & Williamson's model [42], Cooper, Mikic, and Yovanovich's model [44], Mikic's model[43], ICARUS models[55], Person's model[56] Majumdar and Bhushan model [57], etc.
2. A force is applied; due to the contact surface, the material exerts tangential and normal pressure in the contact region. Due to the pressure, the material develops stresses and undergoes structural changes if the stress exceeds the limit.
3. Due to the external forces and internal pressure, both surfaces in contact develop stresses and strain, which means that both surfaces undergo deformation. Due to this, the computation of the displacements is relative. Two approaches have been performed in the literature.
 - (a) Direct approach to compute deformation at each surface in contact using FEM-BEM approaches.
 - (b) Composite approach where the displacement of one of the surfaces is fixed, whereas relative displacement of the other surface with respect to the fixed one is computed. This method offers two advantages: (i) the computational cost of the system is cheaper, and (ii) the ability to include complex surfaces. In this approach, a complex structure is smoothed out via a linear/non-linear map; later, after realizing the displacement, strains, and stresses, the mapping is reversed to understand the system comprehensively.
4. "Mechanical wear is a result of mechanical action ."Due to the material actions, wear develops over a number of cycles of repeated wear, and the materials get removed. It can be seen that material removal rate (ω) is directly proportional to (a) sliding distance(S), (b) normal pressure(P_n), (c) a dimensionless wear coefficient(K), and (d) inversely proportional to surface hardness(H)

i.e.

$$\omega = K \frac{P_n \cdot S}{H} \quad (3.20)$$

The expression in Eqn. 3.20 is referred to as Archard wear law. Nowadays, many such laws consider different aspects of wear, the details of which have to be connected with the physics of material deformation (1), (2), and (3). With these in the forthcoming sections, we first develop the method for wear depth predictions and comment more on wear laws. A numerical model is presented in a variational approach, incorporating rough surfaces' complex topography and micro-macro coupling. Later, the implementation of a finite element of the total model is discussed in detail.

3.1.4 Mathematical Formulation

(a)Wear depth predictions

The variational methods of contact require the definition of bodies under consideration, the contact region between them, strain and stress acting on them, and friction considerations between them. Moreover, an energy consideration has to be considered. From a contact perspective, the forces acting on the contact surface, considering the rough profile, must be considered. We can then construct the finite element formulation that includes the roughness profile based on the energy consideration. This section provides an indicative prediction of wear depth. In contrast, a more general formulation regarding the variational methods to wear is presented in the upcoming section, incorporating the wear depth from this section. When two materials are in contact and have friction, the amount of material gets removed from the surface. The amount of material removed is referred to as wear depth. Wear depth can be numerically estimated using the wear profile. Wear profile is a function of depth with respect to the position at the region where the surfaces come into contact. As the materials get removed, the wear profile changes and a direct comparison between the initial and final profiles indicates wear.

Measurement of the wear profiles can be seen in Moore [66], Sato [67], Olofsson, and Telliskvi [68], in rails and rail wheels. See also Hills and Nowell [69], Arakere and Swanson [70], Vingsbo et. al. [71] on fretting wears.

To formalize, wear is formulated in the related literature with respect to the change in the following quantities [41]

1. Mass of material removed from solid.

2. Reduction of volume in the material.

3. Reduction in dimension of the body, Kennedy and Ling [72] suggested wear rate a function of normal pressure, sliding velocity and temperature. In the case of abrasion, the wear rate is proportional to frictional force.

Let A and B be two bodies under frictional contact whose domain is $\Omega_A \in \mathbb{R}^N$ and $\Omega_B \in \mathbb{R}^N$. Define a vector-valued displacement of the body $\mathbf{u}(\mathbf{X}, t) : \Omega \times [0, t] \rightarrow \mathbb{R}^3$, for a position vector $\mathbf{X} \in \Omega$ and t being pseudo time in quasi-static, and time in dynamics setting. Consequently, for a position vector ($\mathbf{X} \in \Omega_A, \mathbf{X} \in \Omega_B$), deformation vectors are defined as $(\mathbf{u}_A, \mathbf{u}_B)$. Let $\partial\Omega_A$, and $\partial\Omega_B$ be delimiting boundaries of Ω_A , and Ω_B respectively, then it is assumed that the velocities $(\mathbf{v}_c^+, \mathbf{v}_c^-)$ describes the wearing out boundaries on $(\partial\Omega_A, \partial\Omega_B)$ respectively, mainly due to

1. deformation of the bodies $(\mathbf{v}_A, \mathbf{v}_B)$,
2. wear process $(\mathbf{v}^+, \mathbf{v}^-)$.

Note that $(\mathbf{v}_A, \mathbf{v}_B)$ are nothing but material velocities. Let ρ_A and ρ_B be mass densities, and m_A and m_B describe the rate of mass flowing out of boundaries $\partial\Omega_A$ and $\partial\Omega_B$ due to wear process respectively. Then the relationship between the mass (m_A, m_B) and the velocities $(\mathbf{v}_A, \mathbf{v}_B)$ can be written as

$$\begin{aligned} m_A &= \rho_A(\mathbf{v}_A - \mathbf{v}_c^+) \cdot \mathbf{n}^+ = -\rho_A \mathbf{v}^+ \cdot \mathbf{n}^+ \\ m_B &= \rho_B(\mathbf{v}_B - \mathbf{v}_c^-) \cdot \mathbf{n}^- = -\rho_B \mathbf{v}^- \cdot \mathbf{n}^-, \end{aligned} \quad (3.21)$$

where $\mathbf{n}^+$ and $\mathbf{n}^-$ are unit normal vectors to the boundaries $\partial\Omega_A$ and $\partial\Omega_B$ respectively. Notice that the term $(\mathbf{v}_A - \mathbf{v}_c^+)$ is the difference between the material velocities and wearing out of boundary leading to the velocity of the material left subjected to wear. Consequently, wear at the boundaries can be then defined as $\mathbf{v}^+ \cdot \mathbf{n}^+ = v^+$ for $\partial\Omega_A$, and $\mathbf{v}^- \cdot \mathbf{n}^- = v^-$ $\partial\Omega_B$.

Galin and Goryacheva [41] assumed that normal pressure and sliding velocities constitute the velocity of wearing out of the solids under contact. Consequently, Rabinowicz [73] defines this process within the context of Greenwood's theory that $\mathbf{v}^+$ defines the velocity at which $\partial\Omega_A$ travels into surface $\partial\Omega_A$ due to wear. See Fig. 34(a) for a kinematic wear description. Within the context of Eulerian description of displacement functions $(\mathbf{u}_A, \mathbf{u}_B)$, the velocities of the displacement (deformation) $(\mathbf{v}_A, \mathbf{v}_B)$ are related as:

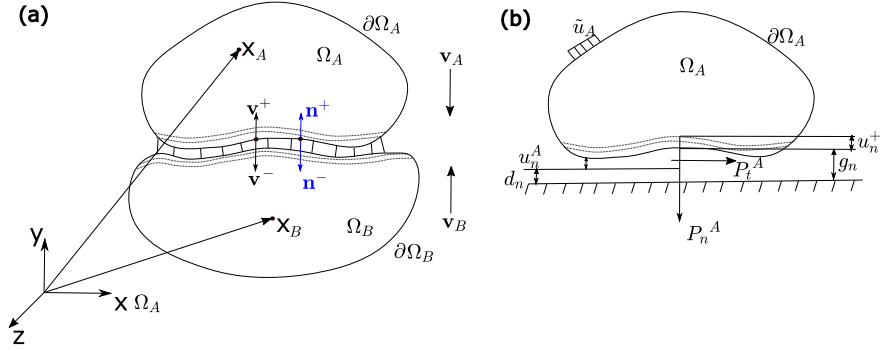


Figure 34: (a) Kinematics of wear profile wearing out at the boundaries of the solid, (b) Quantities defining wear depth (u_n^+), initial gaps g_n , normal and tangential forces (P_n^A , P_t^A), gaps between the contact bodies d_n .

$$\mathbf{v}_A = \frac{d\mathbf{u}_A}{dt} = \dot{\mathbf{u}}_A \quad \mathbf{v}_B = \frac{d\mathbf{u}_B}{dt} = \dot{\mathbf{u}}_B. \quad (3.22)$$

Consequently, the relative sliding velocities of two bodies $\mathbf{V}_{AB}$ can be written in terms of the rate of change of displacements as:

$$\mathbf{V}_{AB} = (1 - \mathbf{n}^+ \otimes \mathbf{n}^+)(\dot{\mathbf{u}}_A - \dot{\mathbf{u}}_B), \quad (3.23)$$

$$= (1 - \mathbf{n}^+ \otimes \mathbf{n}^+)(\mathbf{v}_A - \mathbf{v}_B), \quad (3.24)$$

where $\otimes$ represents the dyadic product.

The total gap (d_n) between two bodies as in Fig. 34(b) can be defined as the sum of initial gap (g_n), the differences in the elastic deformations of two bodies (u_n^A , u_n^B) and the depth of the wear (u_n^+ , u_n^-) as:

$$d_n = g_n - (u_n^A - u_n^B) + (u_n^+ - u_n^-); \quad \text{on } \partial\Omega_A \cup \partial\Omega_B \quad (3.25)$$

where the elastic deformations of each body at the boundary can be written as:

$$\begin{aligned} u_n^A &= (\mathbf{n}^+ \otimes \mathbf{n}^+) \mathbf{u}_A = u_n^A \mathbf{n}^+ \quad \forall \mathbf{x}_A \in \partial\Omega_A \\ u_n^B &= (\mathbf{n}^- \otimes \mathbf{n}^-) \mathbf{u}_B = u_n^B \mathbf{n}^- \quad \forall \mathbf{x}_B \in \partial\Omega_B. \end{aligned} \quad (3.26)$$

The total depth of the material removed (u_n^+ , u_n^-) over a period of time $[0, t]$

can be defined using the velocities as:

$$\begin{aligned} u_n^+ &= \int_0^t v^+(\mathbf{x}, \tau) d\tau \quad \forall \mathbf{x} \in \partial\Omega_A \\ u_n^- &= \int_0^t v^-(\mathbf{x}, \tau) d\tau \quad \forall \mathbf{x} \in \partial\Omega_B \end{aligned} \quad (3.27)$$

Fig. 34(b) shows the principle quantities that define wear depth.

Contact problems require stress and strain to be computed within the solids. Moreover, velocity and stress at the contact region must be calculated. Naturally, physical conditions have to be met, such as (a) non-penetrating property (bodies cannot penetrate), (b) separated from each other (no tensile normal force), which translates to

1. the total normal gaps are always greater (when not in contact) or equal to (during contact) zero

$$dn \geq 0 \quad \forall \mathbf{x} \in \partial\Omega_A, \quad (3.28)$$

2. the tensile normal force is less than (when not in contact) or equal to (during contact) zero

$$p_n^A \leq 0 \quad \forall \mathbf{x} \in \partial\Omega_A. \quad (3.29)$$

Then, contact force $\mathbf{P}_A$, normal force $\mathbf{P}_n^A$, and tangential tractions $\mathbf{P}_t^A$ of solid A can be written as:

$$\begin{aligned} \mathbf{P}_A &= \boldsymbol{\sigma}_A \mathbf{n}^+ \quad \text{on } \partial\Omega_A \\ \mathbf{P}_n^A &= (\mathbf{n}^+ \otimes \mathbf{n}^+)(\boldsymbol{\sigma}_A \mathbf{n}^+) \equiv \mathbf{P}_n^A \mathbf{n}^+ \\ \mathbf{P}_t^A &= (1 - \mathbf{n}^+ \otimes \mathbf{n}^+)(\boldsymbol{\sigma}_A \mathbf{n}^+) \end{aligned} \quad (3.30)$$

where $\boldsymbol{\sigma}_A = \mathbb{C} : \boldsymbol{\varepsilon}_A$ is the Cauchy stress tensor, $\mathbb{C}$ is the constitutive (elasticity tensor) relationship and $\boldsymbol{\varepsilon}$ is the deformation gradient of the displacement $\mathbf{u}$ in the body A defined as:

$$\boldsymbol{\varepsilon}(\mathbf{u}) = \frac{1}{2}(\nabla \cdot \mathbf{u} + \nabla^T \cdot \mathbf{u}). \quad (3.31)$$

In the presence of friction with friction coefficient μ , the tangential traction satisfies,

$$|\mathbf{P}_t^A| \leq \mu_A |\mathbf{P}_n^A|, \quad (3.32)$$

and the slip condition

$$\mathbf{P}_t^A = -\mu_A |\mathbf{P}_n^A| \frac{\mathbf{V}_{AB}}{|\mathbf{V}_{AB}|}. \quad (3.33)$$

The above relationships, subjected to the Dirichlet and Neumann boundary conditions, can compute the model's tangential and normal tractions via displacements and displacement gaps. These tangential and normal tractions can be used to calculate the wear rate via wear law, which is discussed in detail in the sequel.

Archard [74] formulated that the volume of material removed (ω) is directly proportional to normal pressure (P_n), wear coefficient (K), sliding distance (S) and inversely proportional to hardness (H), i.e.,

$$\omega = K \frac{P_n \cdot S}{H}. \quad (3.34)$$

The dimensionless wear coefficient (K) in Eq. (3.34) can be defined in different ways based on a physical model. From the thermodynamics point of view, for E_A energy consumed by the formation of unit mass m_A of wear debris, the following inequality has to satisfy:

$$m_A E_A \geq 0, \quad m_B E_B \geq 0, \quad (3.35)$$

meaning that internal energy spent during the wear process is non-negative.

3.1.5 Variational Methods to Wear

In this section, the constitutive initial boundary value problem is developed based on the thermodynamic and energy considerations of the contact problem with embedded roughness. Embedded roughness is introduced via composite topography as in [45, 65].

Governing Equation and Strong Form

Consider two deformable bodies having its domains $\Omega_i \in \mathbb{R}^n$ ($i=1, 2$), with its external boundary $\partial\Omega_i \in \mathbb{R}^{n-1}$. Furthermore, the external boundary of each body $\partial\Omega_i$ comprises of Dirichlet part $\partial\Omega_i^D$ and Neumann part, $\partial\Omega_i^N$, such that $\bigcup_i(\partial\Omega_i^D \cup \partial\Omega_i^N) = \partial\Omega$ and $\partial\Omega_i^D \cap \partial\Omega_i^N = \emptyset$. We can define a position vector $\mathbf{x} \in \Omega_i$, and a vector valued displacement function of the body $\mathbf{u}(\mathbf{x}, t) : \Omega \times [0, t] \rightarrow \mathbb{R}^3$. On the boundaries, a Dirichlet condition corresponding to the displacement of $\bar{\mathbf{u}}_i(\mathbf{x})$ can be applied for all $\mathbf{x} \in \partial\Omega_i^D$ for each i , and a Neumann condition corresponding to traction of $\bar{\mathbf{t}}_i(\mathbf{x})$ can be applied for all $\mathbf{x} \in \partial\Omega_i^N$.

The two bodies Ω_i are in contact, and the region of the contact is defined with $\Gamma \in \mathbb{R}^{n-1}$, where opposite boundaries Γ_i ($i=1, 2$) of two bodies are considered to be in contact, i.e. $\Gamma = \bigcup_{i=1,2} \Gamma_i$. The contact region in the interface Γ_i is represented by

Γ^c with $\Gamma^c = \Gamma_1^c \cup \Gamma_2^c$, where Γ_i^c ($i=1, 2$) is the region in body (1, 2) in contact. The region Γ_i^c is normally known a priori. The distinction between Γ_i^c and Γ_i is allowed for two reasons. (a) External crack sets such as Γ_i^{ext} is allowed in the framework. (b) The interface Γ_i is normally flat but microscopically embeds a rough profile. Here, Γ_i ($i=1,2$) is allowed to be the same or negative of each other without any restrictions. If the roughness of the surface is embedded into the contact area, then the contact region is a subset of the total area under consideration. i.e., $\Gamma_i^c \subset \Gamma_i$.

A curvilinear coordinate system is introduced to introduce roughness into the profile. Let $\xi_i = \xi(\mathbf{x})$ be a map that establishes a one-to-one correspondence with respect to the global reference system $\mathbf{x} \in \mathbb{R}^n$ in the interface. The rough profile embedded in Γ_i is transformed into a smoother profile using the curvilinear setting; hence the i^{th} rough profile smoother representation is given by $\bar{h}_i(\xi_i)$ as in Fig. 35(b). A unit tangential and normal vector $\mathbf{t}_i(\xi)$ and $\mathbf{n}_i(\xi)$ pointing outwards from domain Ω_i can be defined to compute the tangential and normal forces at the contact surfaces. Along the smoothed curve, at any point ξ , a direction can be identified to represent the smoothed curve $\bar{h}_i(\xi_i)$ as in Fig. 35(b).

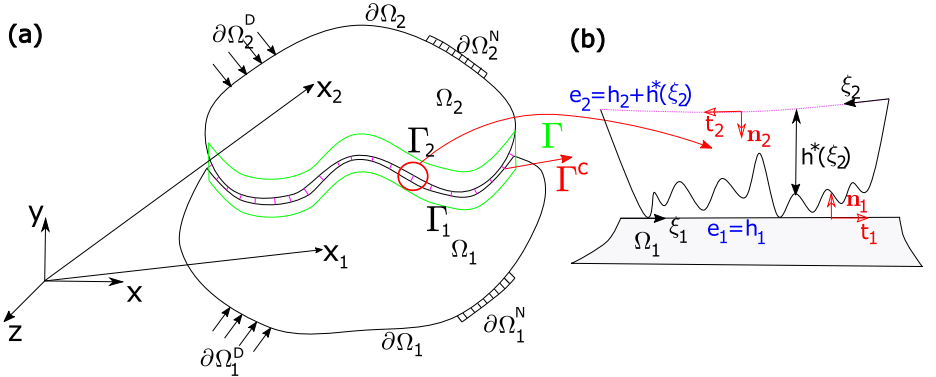


Figure 35: (a) Definition of two deformable bodies under contact, (b) Composite topography of the interface with embedded roughness.

Two assumptions were made in the above section: (a) the rough profile is smoothed out, and (b) the interface subjected to contact can be defined using a one-dimensional mapping function ξ . Consequently, actual elevation considering the rough profile needs to be computed for a realistic argument; hence, considering the rough profile, the actual elevation $e_i(\xi_i)$ can be described in the curvilinear setting as the combi-

nation of the smoothed curve $\bar{h}_i(\xi_i)$ and the roughness function $h_i(\xi_i)$ as:

$$e_i(\xi_i) := \bar{h}_i(\xi_i) + h_i(\xi_i) \quad (3.36)$$

With such a definition at hand and smoothed profiles parallel, the unit vector's tangential and normal vectors are equal and opposite. i.e.:

$$t_1(\xi_1) = 1 - t_2(\xi_2) \text{ and } n_1(\xi_1) = -n_2(\xi_2). \quad (3.37)$$

Furthermore, instead of handling two dissimilar elastic bodies, with each having a roughness profile, as a simplification, two dissimilar elastic bodies with a boundary are replaced by an arbitrary geometry whose roughness profile is the sum of the total roughness of the dissimilar elastic bodies indenting an elastic half plane, using the idea called composite topography. See Fig. 35(b) for more details.

This framework introduces a common coordinate at the local setting ξ . The composite topography Γ^* of interface represented by a flat curve, $e_2 = \bar{h}_i(\xi)$ and a profile with composite roughness $e_1(\xi) = \bar{h}_2(\xi) + h^*(\xi)$ representing an indenter profile, where $h^*(\xi) := \max[\bar{h}_1(\xi) + h^*(\xi)]$, as shown in Fig. 35(b)

Such a transformation can introduce a cohesive zone-like layer with zero thickness. Consequently, a roughness profile can be attached to this interface to represent the composite topography. Consequently, a zero thickness interface model for Γ^* is introduced and defined by two initially co-incident curves described by $h^*(\xi)$ and $e_2(\xi)$. Also, notice that in the general setting, $h^*(\xi)$ and $e_2(\xi)$ are enough to represent the complex rough profile along with transformations. This composite topography now contains unique tangential (**t**) and normal (**n**) unit vectors computed at any point of the surface. For $\mathbf{X} \in \mathbb{R}^n$, the body is characterized by kinematic displacement field, $\mathbf{u}(\mathbf{x}) : \Omega \rightarrow \mathbb{R}^n$. Assuming enough regularity at the interface, let $\mathbf{u}_i = (u_i, v_i, \omega_i)^T$ maps the transformation from undeformed to deformed one and vice versa. Then, a finite strain tensor, ε_i is defined as the symmetric part of displacement gradient $\varepsilon_i = \nabla^s \mathbf{u}_i$.

The relative fields at the interface Γ^* are described by relative displacement field $\Delta \mathbf{u} = \mathbf{u}_1 - \mathbf{u}_2$ of the opposite surface of the interface. The displacement gap is further described as the projection of relative displacement $\Delta \mathbf{u}$ into normal and tangential directions. Furthermore, the relative displacement $\Delta \mathbf{u}$ can be further decomposed into relative tangential displacement Δu_t and relative normal displacement Δu_n such that $\Delta \mathbf{u} = (\mathbf{u}_t, \mathbf{u}_n)^T$.

Due to the composite topography framework, the normal gap g_n of the composite profile h^* of the indenter can be computed as a linear combination of the normal

displacement and the composite profile h^* leading to $g_n = \Delta u_n + h^*$. It is more immediate than when $g_n = 0$, the two bodies at a particular point are in contact. On the other hand, $g_n < 0$ would imply penetration of one body into another. Hence, physically, $g_n \geq 0$ is the most suitable restriction in line with the discussion from the previous section. Consequently, a negative normal gap is not permissible so far by definition.

Within the context of the energy of the system, the total energy of the system, within bodies under contact and the interface Γ^* under considerations constitutes the following energies:

1. The external energy Ψ_{ext} due to the applied boundary conditions such as displacement $\bar{\mathbf{u}}$ and traction $\bar{\mathbf{t}}$.
2. Strain energy/elastic generated by the body Ψ_e .
3. Contact energy [free energy of the contact surfaces] Ψ_{cont} .
4. Wear energy associated with wear. Hence, the total pseudo total energy per unit mass per unit volume takes the form:

Consequently, the total pseudo total energy per unit mass per unit volume takes the form:

$$\Pi = \Psi_{ext} + \Psi_e + \Psi_{cont} + \Psi_w \quad (3.38)$$

Furthermore, the essential balance principles driving the wear problem have to satisfy the balance of energy and contact surfaces given by:

$$\rho \dot{e} = \sigma_{ij} \epsilon_{ij} \quad \text{in } \Omega \quad (3.39a)$$

$$\dot{E} = P_n \dot{g}_n + P_t \dot{\omega}_t - P_c \quad \text{on } \Gamma_c \quad (3.39b)$$

where ρ is the mass density of the bulk, $\dot{e}$ is the body's specific energy, and E is the internal energy of the contact surface. Here P_n and P_t are normal contact traction and tangential contact traction respectively. Finally, $\dot{\omega}_t$ presented the the wear rate, whereas $\dot{f} = \frac{df}{dt}$ represents the time derivative.

The Helmholtz free energy density for the linear isotropic material takes the form:

$$\Psi_e(\mathbf{u}) = \frac{1}{2} \boldsymbol{\varepsilon} : \mathbb{C} : \boldsymbol{\varepsilon} = \frac{1}{2} \lambda \text{tr}^2(\boldsymbol{\varepsilon}) + \mu \boldsymbol{\varepsilon} : \boldsymbol{\varepsilon} \quad (3.40)$$

where $\mathbb{C}$ defines the linear elasticity tensor defined as $\mathbb{C} = 2\mu \mathbb{I} + \lambda \mathbf{1} \otimes \mathbf{1}$ in terms of Lamé's constant λ and μ . Here, $\mathbb{I}$ and $\mathbf{1}$ are fourth-order and second-order identity tensors, respectively.

The state laws such as stress can be easily accessible using Helmholtz free energy function as:

$$\sigma := \frac{\partial \Psi}{\partial \varepsilon}. \quad (3.41)$$

At this region of contact, similar to the bulk, a standard Clausius-Duhem inequality for the contact surface satisfies and takes the form:

$$\dot{\Psi} \preceq P_n \dot{g}_n + P_t \dot{\omega}_t \quad \text{on } \Gamma_c \quad (3.42)$$

where Ψ is the internal energy at the interface. The contribution of the internal energy due to contact takes the form:

$$\Psi_{cont} = \int_{\Gamma_c} \frac{1}{2} P_n g_n \cdot g_n \, dS \quad (3.43)$$

Consequently, the wear can be introduced into the model by defining contact force P_n and the gaps, g_n . In other words, the contact pressure P_n is responsible for developing wear. Due to wear, the normal gap g_n changes. As mentioned before, the change in the normal gaps is influenced by two factors. i.e. a) normal displacement Δu_n . stemming from the contact, and b) the roughness of the profile h^* . Furthermore, the wear can be defined using Signorini's contact condition, Coulomb's friction, and Archard's law of wear.

As in the Section 2.2.2, define wear gap ω , for an initial gap of g_0 , between the elastic body and indenter, we have

$$g_n - g_0 \preceq \omega \quad (3.44)$$

Furthermore, state laws that define the contact surface can be written as:

1. Normal pressure cannot be negative, i.e., $P_n \geq 0$.
2. Wear is always less than the difference between the final and initial gaps, i.e., $g_n - g_0 \preceq \omega$.
3. A combination of them would be $P_n(g_n - \omega - g) = 0$. In general, this can be seen as a Karush-Kuhn-Tucker condition.

Notice that P_n is the wear driving force associated with ω . Moreover, the above conditions form the first-order stability conditions with respect to the wear. From the Eq.(3.42)

$$P_n \dot{\omega} + P_t \dot{\omega}_t \geq 0, \quad (3.45)$$

for some relative tangential displacement (ω_t) between the contact surface and the indenter.

Furthermore, the principle of maximum dissipation is used to define Coulomb's law of friction, i.e.:

$$|P_t| \leq \mu(P_n)_+; \quad \omega_t(P_t' - P_t) \leq 0; \quad \forall |P_t| \leq \mu(P_n)_+, \quad (3.46)$$

where μ is a coefficient of friction, $|\cdot|$ stands for the absolute value, and $(P_n)_+ = \frac{(P_n + |P_n|)}{2}$.

Now, the Coulombs law of friction and Archand's law of wear are introduced to evaluate wear rate $\dot{\omega}$ using the normal contact pressure.

$$\dot{\omega} = k(P_n)_+ |\dot{\omega}_t|, \quad (3.47)$$

where k is the wear coefficient constant. Note that the choice $(P_n)_+$ instead of P_n facilitates the use of both $P_n \geq 0$ and $P_n < 0$. Furthermore, Eq.(3.46) implies that

$$P_t = \mu(P_n)_+ \text{sign}(\dot{\omega}_t) \quad \text{when } \dot{\omega}_t = 0 \quad (3.48)$$

The pseudo-wear energy generated due to wear and friction takes the form,

$$\Psi_w = \int_{\Gamma_c} (k(P_n)_+^2 + \mu(P_n)_+) |\dot{\omega}_t| \quad (3.49)$$

It is clear that $k(P_n)_+^2 |\dot{\omega}_t|$ is the Archand's law of wear used to describe the wear $\dot{\omega}$, where $\mu(P_n)_+ |\dot{\omega}_t|$ is the energy generated due to friction. In the absence of friction, the pseudo-wear energy takes the form:

$$\Psi_w = \int_{\Gamma_c} (k(P_n)_+^2 |\dot{\omega}_t| \quad (3.50)$$

Now, substituting Eq.s (3.47),(3.48),(3.49) into (3.46) leads to the following total pseudo internal energy:

$$\begin{aligned} \pi = \int_{\Omega} \frac{1}{2} \varepsilon : \mathbb{C} : \varepsilon + \int_{\Gamma_c} \frac{1}{2} P_n (g_n) g_n dS \\ + \int_{\Gamma_c} [k(P_n)_+^2 + \mu(P_n)_+] |\dot{\omega}_t| dS + \Psi_{ext} \end{aligned} \quad (3.51)$$

Now, the Eq.(3.51) is solved for displacement $\mathbf{u}$ and relative displacement $\Delta \mathbf{u}$. Later the actual gap g is estimated using composite topography,

$$\mathbf{g} = \Delta \mathbf{u} + \mathbf{h}^*, \quad (3.52)$$

Subsequently, wear rate and friction are computed from the primary variable.

Naturally, the solution $\mathbf{u}$ for the total energy functional π at the interface in Eq.(3.51) in the quasi-static setting can be derived by considering the first variation of the functional, i.e.:

$$\delta\pi(\mathbf{u}) = \frac{d}{de}(\mathbf{u} + \mathbf{e}\delta\mathbf{u}) \big|_{e=0} = 0, \quad (3.53)$$

for some text function or a small variation $\delta\mathbf{u}$. For a given initial boundary condition, find $\mathbf{u}$ such that for each $t \in [0, T]$,

$$\begin{aligned} \int_{\Omega} \boldsymbol{\varepsilon}(\mathbf{u}) : \mathbb{C} : \boldsymbol{\varepsilon}(\delta\mathbf{u}) dV + \int_{\Gamma_c} P_n(\Delta\mathbf{u}) g_n(\Delta\delta\mathbf{u}) dS \\ + \int_{\Gamma_c} [k(P_n)_+^2 + \mu(P_n)_+] |\dot{\omega}_t| \delta\mathbf{u} dS = 0 \end{aligned} \quad (3.54)$$

for $\delta\mathbf{u} \in \mathcal{V} := \{\delta\mathbf{u} \in H(\Omega) \times [0, T]; \delta\mathbf{u} = 0 \text{ on } \partial\Omega_{\mathbf{u}}\}$

3.2 Finite Element Implementation

The numerical treatment to solve the weak equation Eq.(3.54) involves introducing a finite element for the bulk Ω and the interface Γ . Notice that Ω is subdivided into Ω_1 and Ω_2 due to the contact.

First, the Finite Element (FE) implementation of the bulk is presented briefly; later, the FE of the interface is presented. Define the discretization of the bulk $\Omega \rightarrow \Omega_i^h$ and the interface $\Gamma \rightarrow \Gamma^h$ for some discrete mesh $\mathbf{h}$ such that partition of unity and the compactness of the isoparametric function in Ω_i^h and Γ^h is maintained. The displacement field $\mathbf{u}$ and the strain $\boldsymbol{\varepsilon}$ are interpolated in terms of the nodal displacement $\mathbf{d}$ as follows,

$$\mathbf{u}(\mathbf{x}) = \mathbf{N}(\mathbf{x})\mathbf{d} \quad \boldsymbol{\varepsilon} = \mathbf{B}(\mathbf{x})\mathbf{d} \quad (3.55)$$

where $\mathbf{N}(\mathbf{x})$ is the matrix that contains the shape function, and $\mathbf{B}(\mathbf{x})$ defines its corresponding spatial derivative. Similarly, the test function $\delta\mathbf{u}$ and the corresponding strain $\boldsymbol{\varepsilon}(\delta\mathbf{u})$ takes the form,

$$\delta\mathbf{u}(\mathbf{x}) = \mathbf{N}(\mathbf{x})\delta\mathbf{d}; \quad \boldsymbol{\varepsilon}(\delta\mathbf{u}) = \mathbf{B}(\mathbf{x})\delta\mathbf{d} \quad (3.56)$$

The insertion of the interpolation scheme into the weak form leads to the following discrete residual.

$$\mathbf{R}^u = \int_{\Omega} \mathbf{B}^T : \boldsymbol{\sigma} dV - \int_{\Omega_u} \mathbf{N}^T \cdot \mathbf{f}_v dV - \int_{\partial\Omega} \mathbf{B}^T \cdot \bar{\mathbf{t}} dS. \quad (3.57)$$

Moreover, the stiffness leads to:

$$\mathbf{K}_{uu} = \frac{\partial \mathbf{R}^u}{\partial \mathbf{d}} = \int_{\Omega} \mathbf{B}^T \mathbb{C} \mathbf{B} dV. \quad (3.58)$$

Then, the finite element approximation of bulk takes the form

$$\mathbf{K}_{uu} \cdot \mathbf{d} = \mathbf{R}^u \quad (3.59)$$

where the above equation is solved for $\mathbf{d}$ using a system of linear equations.

At the interface Γ^h , a conforming finite element discretization for the continua is assumed. The interpolation of the interface is carried out by the displacement field $\mathbf{u}$ of the bulk in the discrete domain Ω .

Consequently, the interface finite element with embedded toughness is introduced, capable of handling wear and friction.

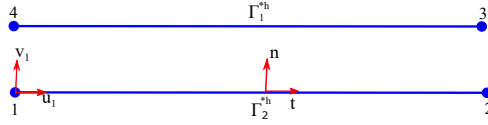


Figure 36: Interface finite element topology

Let $\mathbf{d}$ be the collection of generalized displacement for the four-node interface as

$$\mathbf{d} = \{u_1, v_1, u_2, v_2, u_3, v_3, u_4, v_4\}^T \quad (3.60)$$

The contribution of the interface from the weak form can be realized as,

$$\int_{\Gamma_c} P_n(\Delta \mathbf{u}) g_n(\Delta \delta \mathbf{u}) dS + \int_{\Gamma_c} [k(P_n)_+^2 + \mu(P_n)_+] |\dot{\omega}_t| \delta \mathbf{u} dS \quad (3.61)$$

which can be interpolated as

$$\int_{\Gamma_c} P_n(\Delta \mathbf{u}) g_n(\Delta \delta \mathbf{u}) dS \approx \mathbf{A}_{e=1}^{nel} \lim \int_{\Gamma_c^h} P_n(\Delta \mathbf{u}) g_n(\Delta \delta \mathbf{u}) dS \quad (3.62)$$

and

$$\int_{\Gamma_c} [k(P_n)_+^2 + \mu(P_n)_+] |\dot{\omega}_t| \delta \mathbf{u} \, dS \approx \mathbf{A}_{e=1}^{nel} \lim \int_{\Gamma_c^h} [k(P_n)_+^2 + \mu(P_n)_+] |\dot{\omega}_t| \delta \mathbf{u} \, dS \quad (3.63)$$

Here subscript 'e' refers to the e^{th} interface element such that $e \in \{1, \dots, nel\}$ and ' $\mathbf{A}$ ' refers to symbolic assembly operator. The integral in the above equation can be computed using the two-point Newton-Cotes quadrature formula.

A local reference system of tangential vector $\mathbf{t}$ and normal vector $\mathbf{n}$ is defined as in the figure, with its origin 'O' in the local reference plane placed at the centre. Hence, the rotation matrix $\mathbf{R}$ is pre-multiplied. The relative displacement $\delta \mathbf{u}$ is then computed as,

$$\Delta \mathbf{u} = \mathbf{R} \mathbf{N} \mathbf{L} \mathbf{D} \quad (3.64)$$

where the operators $\mathbf{R}$, $\mathbf{L}$ and $\mathbf{N}$ are defined as

$$\mathbf{R} = \begin{bmatrix} tx & ty \\ nx & ny \end{bmatrix} \quad (3.65)$$

is the local rotation matrix

$$\mathbf{L} = \begin{bmatrix} -1 & 0 & 0 & 0 & 0 & 0 & +1 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & +1 \\ 0 & 0 & -1 & 0 & +1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & +1 & 0 & 0 \end{bmatrix} \quad (3.66)$$

estimates the relative displacement between the upper and lower sides of the interface Γ_{c1}^* and Γ_{c2}^* .

The shape function $\mathbf{N}$ now takes the form:

$$\mathbf{N} = \begin{bmatrix} N1 & 0 & N2 & 0 \\ 0 & N1 & 0 & N2 \end{bmatrix} \quad (3.67)$$

with $N_1 = (\frac{1-\xi}{2})$ and $N_2 = (\frac{1+\xi}{2})$ are linear shape function. Here ξ is the local coordinate system such that $\xi \in [0,1]$ in each element.

Once $\Delta \mathbf{u} = (\Delta u_t, \Delta u_n)^T$ is computed, this cannot be considered as an actual gap. Moreover, computed gaps need to account for the roughness of the profile. Consequently, actual normal gap g_n and tangential gap g_t is modified to account for the roughness profile as:

$$g_n = \Delta u_n + h^* \quad g_t = \Delta u_t + h^* \quad (3.68)$$

Moreover, to consider wear due to the sliding motion stemming from the tangential gaps Δu_t , and the wear stemming from the normal gaps Δu_n , a quantity defined as "separation" $\mathcal{S}$ is introduced. The easiest choice for the separation function that includes the tangential and normal gaps can be based on the L^2 norm of the gap functions, i.e.:

$$\mathcal{S} = ((\Delta u_t)^2 + (\Delta u_n)^2)^{\frac{1}{2}} \quad (3.69)$$

Moreover, due to the composite topography framework introduced to include the rough profile, the separation can be modified either as

$$\mathcal{S} = ((g_t)^2 + (g_n)^2)^{\frac{1}{2}} \quad (3.70)$$

or as

$$\mathcal{S} = ((\Delta u_t)^2 + (\Delta u_n)^2)^{\frac{1}{2}} + f(h^*) \quad (3.71)$$

Here, $f(h^*)$ represents the updated profile due to the wear. The function $f(h^*)$ is updated at each increment to consider the model's wear rate. Eq. 3.71 is chosen in the current consideration due to easy manipulations of the gradient term. Consequently, normal traction P_n is estimated as:

$$P_n = \begin{cases} K\mathcal{S}, & \text{if } g_n > 0. \\ 0, & \text{if } g_n \leq 0. \end{cases} \quad (3.72)$$

whereas the tangential traction P_t stemming from the sliding motion can be defined as:

$$P_t = \mu P_n \tanh \left\{ \frac{\Delta u_t - f \cdot \Delta u_t}{\varepsilon_T} \right\} \quad (3.73)$$

Here, the function f and ε_T are properties related to the geometry of the indenter whose details are presented in the sequel. μ corresponds to the coefficient of friction between the bodies under contact.

Notice that due to the Eq. 3.71, the following conditions arise. When the Normal gaps $(\Delta u_t) = 0$, the two bodies are not in contact, hence, upon applying any load in the tangential direction leads to the $\mathcal{S} > 0$. But when both the normal and tangential loads are applied, Eq. 3.71 presents the combined effects of both loads.

Furthermore, when the tangential load is absent, the normal pressure P_n in Eq. (3.72) coincides with [45]. Consequently, to avoid the redundancy issue with the tangential force, an extra condition such as $P_n = K\mathcal{S}$ if and only if $g_n > 0$. Furthermore, this allows for an effective combination of the tangential load in a normal pressure. Furthermore, normal pressure P_n leads to micro-scale interaction due to contact coming from the bulk.

The discrete residual is then computed as:

$$\mathbf{R}_e^{(k)} = \int_{\Gamma_c} \mathbf{L}^T \mathbf{N}^T \mathbf{R}^T \mathbf{P} \, d\mathbf{A} \quad (3.74)$$

with $\mathbf{P} = (P_t, P_n)$ are tangent vectors, and the stiffness matrix for the interface reads

$$\mathbf{K}_e^{(k)} = \int_{\Gamma_c} \mathbf{L}^T \mathbf{N}^T \mathbf{R}^T \mathbb{C}_c \mathbf{R} \mathbf{N} \mathbf{L} \, d\mathbf{A} \quad (3.75)$$

with the linearized constitutive matrix $\mathbb{C}_c$ takes the form:

$$\mathbb{C}_c = \begin{bmatrix} \frac{\partial P_t}{\partial g_t} & \frac{\partial P_t}{\partial g_n} \\ \frac{\partial P_n}{\partial g_t} & \frac{\partial P_n}{\partial g_n} \end{bmatrix}. \quad (3.76)$$

The particular expression for the $\mathbb{C}_c$ takes the form

$$\frac{\partial P_t}{\partial g_t} = \frac{P_n}{\varepsilon_T} \left[1 - \tanh^2 \left(\frac{g_t - f * \dot{g}_t}{\varepsilon_T} \right) \right] \quad (3.77)$$

$$\frac{\partial P_t}{\partial g_n} = \frac{2 * \mu K}{\mathcal{S}} \Delta u_t \tanh \left(\frac{g_t - f * \dot{g}_t}{\varepsilon_T} \right) \quad (3.78)$$

$$\frac{\partial P_n}{\partial g_t} = \frac{2K g_t}{\mathcal{S}} \quad (3.79)$$

$$\frac{\partial P_n}{\partial g_n} = \frac{2K g_n}{\mathcal{S}} \quad (3.80)$$

$$(3.81)$$

For the friction-less normal contact, the linearized constitutive matrix reads:

$$\mathbb{C}_c = \begin{bmatrix} 0 & 0 \\ 0 & \frac{\partial P_n}{\partial g_n} \end{bmatrix} \quad (3.82)$$

The contribution from the energy created/ dissipated due to wear, as in Eq. (3.89), can be written as:

$$\int_{\Gamma_c} [k(P_n)_+^2 + \mu(P_n)_+] |\dot{\omega}_t| \delta \mathbf{u} \, dS \quad (3.83)$$

with $\dot{\omega}_t = \dot{g}_t = \frac{(g_t - g_{t-1})}{dt}$, the above expression can be discretised using the Finite element created in this section for the interface element as:

$$\mathbf{R}_w^{(k)} = \int_{\Gamma_c} \mathbf{L}^T \mathbf{N}^T \mathbf{R}^T \mathbf{P}_w \, dA \quad (3.84)$$

with $\mathbf{P}_w = (P_t^w + P_n^w)$ are tangent vectors, and the stiffness matrix due to the wear for the interface reads:

$$\mathbf{K}_w^{(k)} = \int_{\Gamma_c} \mathbf{L}^T \mathbf{N}^T \mathbf{R}^T \mathbb{C}_w \mathbf{R} \mathbf{N} \mathbf{L} \, dA \quad (3.85)$$

with the linearized constitutive matrix $\mathbb{C}_w$ takes the form:

$$\mathbb{C}_w = \begin{bmatrix} \frac{\partial P_t^w}{\partial g_t} & \frac{\partial P_t^w}{\partial g_n} \\ \frac{\partial P_n^w}{\partial g_t} & \frac{\partial P_n^w}{\partial g_n} \end{bmatrix} \quad (3.86)$$

Moreover, the tangential and the normal force due to wear can be written as:

$$P_t^w = \mu(P_n)_+ |\dot{g}_t| \quad (3.87)$$

$$P_n^w = 2K(P_n)_+^2 g |\dot{g}_t| \quad (3.88)$$

whereas the rate of wear $\dot{W}_n$ due to the normal force can be written using the Archard wear law, which reads

$$\dot{W}_n = K(P_n)_+^2 |\dot{g}_t|. \quad (3.89)$$

Here, $(P_n)_+ = \frac{P_n + |P_n|}{2}$. Furthermore, particular expressions for the tangents due to wear can be computed as:

$$\frac{\partial \mathbf{P}_t^w}{\partial \mathbf{g}_t} = \mu(\mathbf{P}_n)_+ \frac{1}{dt} \quad (3.90)$$

$$\frac{\partial \mathbf{P}_t^w}{\partial \mathbf{g}_n} = 2\mu K |\dot{\mathbf{g}}_t| \quad (3.91)$$

$$\frac{\partial \mathbf{P}_n^w}{\partial \mathbf{g}_t} = 2K(\mathbf{P}_n)_+^2 \frac{1}{dt} \quad (3.92)$$

$$\frac{\partial \mathbf{P}_n^w}{\partial \mathbf{g}_n} = 6K^2(\mathbf{P}_n)_+ |\dot{\mathbf{g}}_t| \quad (3.93)$$

$$(3.94)$$

Consequently, the total elemental stiffness and the residuals are a linear combination of the stiffness and residual stemming from the contact and wear process.

$$\mathbf{R}^{(k)} = \int_{\Gamma_c} \mathbf{L}^T \mathbf{N}^T \mathbf{R}^T \mathbf{P} \, d\mathbf{A} + \mathbf{P}_w \quad (3.95)$$

with $\langle \mathbf{P} \rangle + \mathbf{P}_w$ are residual values added appropriately, and the stiffness matrix due to the combined effects of contact and wear for the interface reads

$$\mathbf{K}^{(k)} = \int_{\Gamma_c} \mathbf{L}^T \mathbf{N}^T \mathbf{R}^T (\mathbb{C}_c + \mathbb{C}_w) \mathbf{R} \mathbf{N} \mathbf{L} \, d\mathbf{A} \quad (3.96)$$

with the linearized constitutive matrix $\mathbb{C}_w$ takes the form,

The resulting algebraic system is solved using a newton-raphson scheme, i.e., solve

$$\mathbf{K}^{(k)} \Delta \mathbf{d} = -\mathbf{R}^{(k)} \quad (3.97)$$

$$\mathbf{d}^{(k+1)} = \mathbf{d}^{(k)} + \Delta \mathbf{d}^{(k)} \quad (3.98)$$

for some iteration 'k' in the Newton-Raphson loop.

Chapter 4

Numerical Simulation

4.1 Introduction

This section proposes benchmark examples to illustrate the efficiency and applicability of the proposed wear model using the MPJR interface finite element problem with embedded roughness. Furthermore, three geometries of similar profiles with cylindrical, flat, and WM function indenters are presented. The specific examples demonstrate the choice of the embedded roughness and their finite element implementation, followed by a detailed assessment of the wear profiles, horizontal and vertical reactions, contour plots regarding the stresses and the displacement, and wear rate. The Finite Element analysis program, FEAP, aims to solve the model using a user-defined Fortran-based subroutine to take advantage of the Newton-Raphson solver.

The present framework considers a flat plate indented using an indenter. Fig. 37 (a) shows the half plane of the flat surface indented by a spherical object. Due to the MPJR framework, the geometries are transformed into two flat blocks and an interface such that the original is fixed at the mid-surface plane of the interface, as shown in Fig. 37 (b). The two blocks of material size of $L = 10\text{mm}$ and height of $h = 5.6\text{mm}$ are shown in Fig. 38 (b). Among these, the lower block (block-2) consists of $h_1 = 5\text{mm}$, and the upper block (block-1) consists of $h_2 = 0.5\text{mm}$. Furthermore, an interface is shared between the blocks with a thickness of $h_i = 0.1\text{mm}$. Moreover, the interface is added to create the desired shape of the indenter, as discussed in Chapter 3

In the present framework, the actual shape of the indenter is embedded into

the flat block via the finite element of the MPJR interface. The profile elevation is computed via the analytical form and evaluated at every Newton-cotes integration point of the interface. Due to the (3.52), the actual gap is the computed gaps' composition and the profile's roughness h^* . The problem is analyzed in plane stress conditions. The lower block is meshed with 200×10 , whereas the upper block is meshed with 200×3 . Unless specified, the interface is meshed with 200 elements, as shown in Fig. 38. The geometry is loaded with a displacement loading condition on the top surface, while the bottom is fixed, as shown in Fig. 37 (b). The details regarding the load history are presented in the sequel. Furthermore, to ensure the rigid body movement between the blocks and the interface. The interface is applied with a tie constant with block-1 and block-2. Consequently, the load applied on block-1 is distributed to block-2 through the interface.

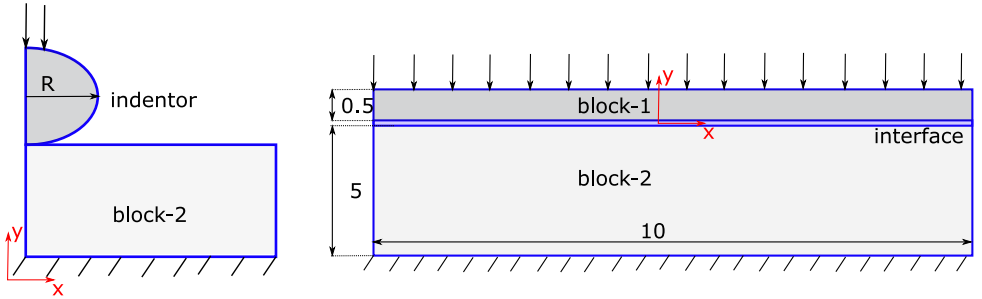


Figure 37: Geometrical description of the contact surface a) original surface, and b) modified geometry with an embedded surface.

Within the context of MPJR theory, two different types of wear can be evaluated. a) a weaker indenter is indenting a more rigid surface, leading to wear in the indenter, and b) a strong indenter is indenting a weaker material. In both cases, the variational framework can capture the wear and friction between them. We aim to understand the wear of the indenter profile. Consequently, the following two approaches can be utilized. a) consider a harder material (such as diamond) for the indenter and with the repeated cycling loading of various weaker materials (such as steel) to understand the wear. This approach can be computationally expensive due to cyclic loading and repeated loading, where other methods include b) a weaker indenter indenting on the harder material, leading to wear on the indenter over a concise load application. In the remainder of this section, approach b) is used to showcase the neat profile. It can be argued that a) is most suitable for

the engineering application, while the physics for cases a) and b) remain the same, justifying case b). Consequently, the indenter block (block-1) is assumed to have Young's modulus of $E_1 = 80000$ MPa and a Poisson's ratio of $\nu_1 = 0.22$. The Lower flat block (block-2) is assumed to have Young's modulus of $E_2 = 210000$ MPa and a Poisson's ratio of $\nu_2 = 0.3$. Notice that, due to the different elastic properties of the two blocks, there is a coupling between normal and tangential contact forces. Furthermore, only normal forces are included in the computation of the wear rate as in Eq. (3.89).

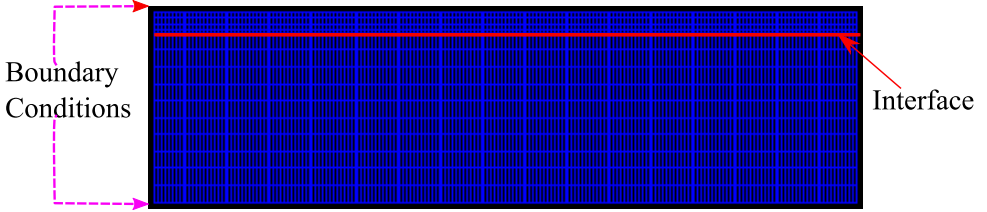


Figure 38: description of the mesh

The interface properties are computed using the composite tomography technique. In this approach, contact constraints involve two linear elastic isotropic materials' relative vertical and horizontal displacements. Consequently, normal tractions exchanged are equal and opposite. Furthermore, the linear elasticity equation for the contact region can be expressed as

$$v_1 - v_2 = \left(\frac{1 - \nu_1^2}{E_1} + \frac{1 - \nu_2^2}{E_2} \right) \frac{P}{\pi r}, \quad (4.1)$$

v_i is the vertical displacement of the interface, r is the radial distance from the contact region, and P is the force applied. Moreover, due to the geometrical transformation presented, the problem can be considered equivalent to the rigid lower block, and the interface is characterized by composite elastic Young's, which takes the form.

$$\frac{1 - \nu^2}{E} = \frac{1 - \nu_1^2}{E_1} + \frac{1 - \nu_2^2}{E_2}, \quad (4.2)$$

whereas the composite shear modulus G takes the form

$$\frac{1 - 2\nu}{G} = \frac{1 - 2\nu_1}{4G_1} + \frac{1 - 2\nu_2}{4G_2}. \quad (4.3)$$

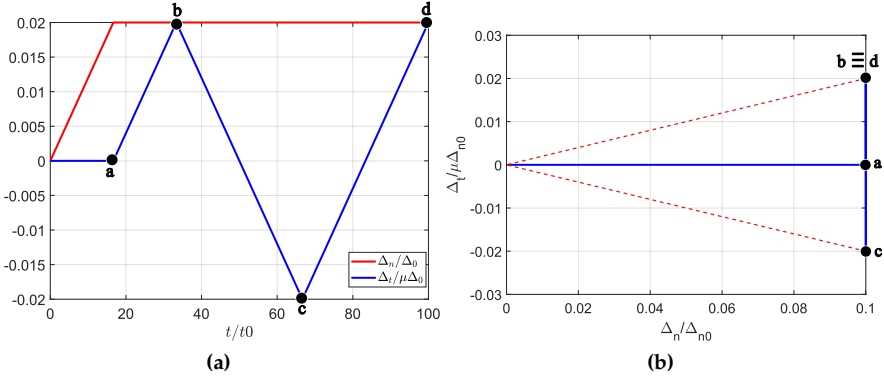


Figure 39: Load histories[75]

Whereas the shear modulus G can be written in terms of Young's modulus as $G_i = \frac{E_i}{2(1 + \nu_i)}$ for $(i = 1, 2)$. Due to the topography, the contacting geometry can be simplified, as shown in Fig. 37 (b).

Regarding the load application, normal and tangential displacement of Δ_n and Δ_t are imposed on the top edge, respectively, as shown in Fig 39 a). Specifically, a normal load (vertically downwards) is applied until a time t and kept constant later on. Meanwhile, a tangential load (horizontal) is applied after the time t as a cyclic load. This ensures contact between the two bodies before any tangential load is applied. Fig 39b) presents the combined imposed displacement in Δ_n, Δ_t space, in which imposed displacements represent the Variation of tangential load with respect to the normal load.

Point (a): The normal load increases monotonically from zero to its maximum value, resulting in both forward slip (positive tangential tractions) and backward slip (negative tangential tractions).

Point (b): Upon the application of the tangential load (point (a) Fig 39, the following events unfold: (i) Tangential tractions increase at the leading contact edge. (ii) Tangential tractions reduce at the trailing contact edge. (iii) Consequently, there will be an abrupt shift from backward slip to adhesion at the trailing edge, followed by the reversal in tractions with an opposing sign. During this process, the adhesive region shrinks, reaching its minimum size at point (b) in the loading sequence.

Point (c): Instantaneously reversing the far-field displacement recreates a stuck region, which dwindles to a minimum at point (c).

Point (d): The system attains a stable state post point (d) with a consistent ad-

hesive area, notably distinct from the initial application for a compliant load. The area remains nearly unchanged in size but shifts towards the centre of the contact region.

First, a spherical indenter is considered in the remainder of this chapter. A detailed analysis of the vertical and horizontal reactions is presented, followed by an analysis of the wear profile. Furthermore, for various indenter radii, a qualitative analysis is performed using dimensionless analysis, followed by a wear profile analysis. Moreover, wear profiles for co-efficient and friction coefficient variations are presented. Furthermore, the rate dependency of the wear profile is elucidated to show the influence of the loading rate on the wear profile. This analysis is later extended to consider a flat indenter. The analysis is extended to the Weierstrass-Mandelbrot (WM) function to feel a realistic engineering surface. Specifically, WM functions up to four harmonics are considered to showcase the reactions and their respective wear profile. The analysis is bolstered by dimensionless analysis of the responses and contour plots regarding the displacement and principle stresses.

4.2 Spherical indenter

In this section, the indenter with the spherical profile is evaluated. The indenter possesses a radius of R ranging from $R = 10\text{mm}$ to $R = 100\text{mm}$ with fixed geometry as in Fig. 37. The boundary conditions and load histories remain the same as previously described. The wear coefficient is $K = 10^{-9}$, and the coefficient of friction is taken as $\mu=0.2$ unless specified. Initially, a vertical displacement is imposed downward on the spherical indenter, and horizontal displacement is imposed in a positive direction, causing it to contact the lower flat plate via the interface. This results in reactions in both directions, leading to interface-induced wear on the interface. The time step is taken as $t_s = 100\text{sec}$, whereas the time increment of $dt = 0.05$ is considered.

The relative displacement between the contacting surfaces is computed as

$$h^* = \sqrt{R^2 - \chi} - \sqrt{R^2 - \chi_y} \quad (4.4)$$

where χ is the radial distance from the contact region, and χ_y is the coordinate at the integration point.

Fig. 40 presents the normal traction P_n at each position on the interface as the time evolves. Furthermore, the x Vs. normal tractions P_n is presented for the indenter radius of $R = 100\text{mm}$ in Fig. 40 (a), and $R = 10\text{mm}$ is in Fig. 40 (b). Notice

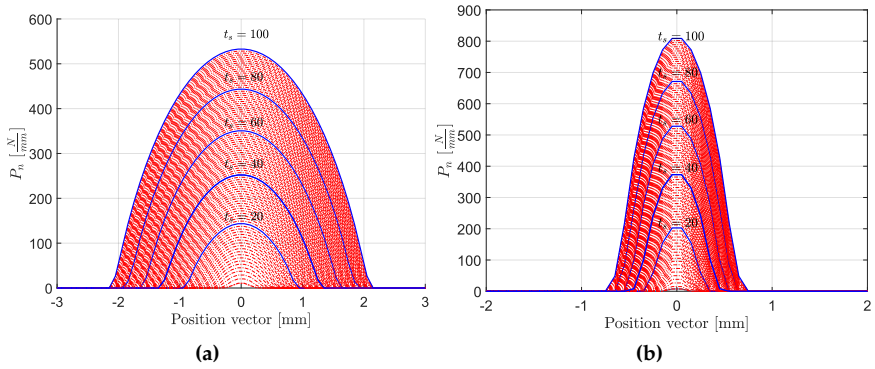


Figure 40: Vertical traction At each position X for the cylindrical impact specimen with a) contact radius of $R = 100\text{mm}$, b) with contact radius of $R = 10\text{mm}$.

that the lower block is dimension $D = 10\text{mm}$ as in Fig. 37 (b). Consequently, the indentation of $R = 10\text{mm}$ will have a smaller curvature than the $R = 100\text{mm}$. This curvature difference also impacts the contact area, as shown in Fig. 40. Fig. 40 also highlights the evolution of the vertical traction as the time t_s increases. In each figure, the evolution at $t_s = 20, 40, 60, 80, 100$ sec are highlighted in blue, whereas the in-between evolution is greyed out using red.

The Fig. 40 showcases several key essential features.

1. The impact of the spherical indenter on the surface can be seen as a point of contact. Due to the initial contact, the contact area associated with the indentation is also small.
2. As the time increases, for example, $t_s = 20$ sec, the contact area grows; consequently, the vertical tractions associated with the interface also increase. This can be seen through the evaluation of the displacement profile.
3. As the radius of the contact area is highly dependent on the radius of the indenter, the vertical traction varies. This can be seen in the difference between the Figs 40a) and b). Notice that the contact area for $R = 10\text{ mm}$ is lower than the $R = 100\text{ mm}$, which can be seen in the figure.
4. As the radius reduces, the vertical traction increases. The total traction force in the case of $R = 100\text{ mm}$ is $P_n = 550\text{ N/mm}$, whereas for the $R = 10\text{ mm}$, the vertical force is found to be $P_n = 800\text{ N/mm}$. This increase could be

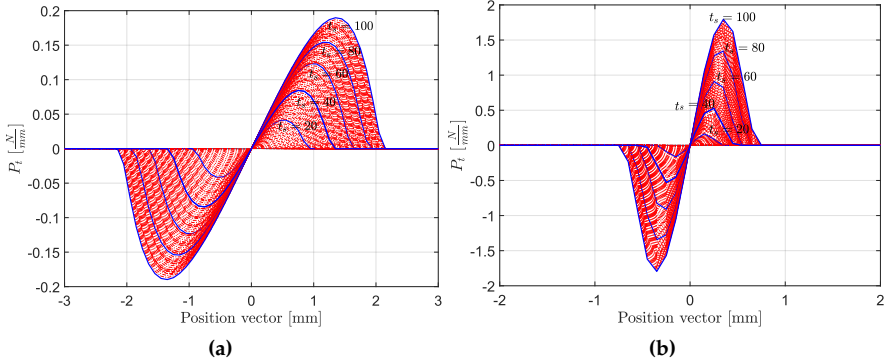


Figure 41: Horizontal traction

attributed to the concentrated force on the smaller area with the same maximum applied displacement.

Due to the loading history in the Δ_t and Δ_n space and the strong coupling in the model, as elucidated in Chapter 3, the horizontal tractions are plotted in the interface at each position. Due to the vertical imposed displacement, the two bodies come in contact. Due to the applied horizontal displacement, tangential tractions increase at the leading edge while diminishing at the trailing edge. Consequently, an abrupt shift from the backward slip to adhesion at the trailing edge, and vice versa on the opposing sign, can be observed in Fig 41. As the load increases, the adhesion region shrinks. Fig 41 presents the evolution of the horizontal/tangential force P_t as the position vector for the radius of $R = 100\text{mm}$ in Fig 41 (a), and $R = 10\text{mm}$, in Fig 41b). Due to the strong coupling and the load sequence, a precise formulation of the slips on both sides can be observed. Moreover, from Fig 41 (a), it can be observed that, as the radius of the indenter increases, the contact area increases, consequently leading to more spread out slips compared to the Fig 41 (b) of radius $R = 10\text{mm}$. Moreover, as in horizontal traction, tangential tractions also increase as the radius of the indenter decreases.

A dimensionless plot is plotted to validate the proposed method with the literature as in [75]. Specifically, The $\frac{x}{x_0}$ Vs. $\frac{P_n}{P_{n,0}}$ or $\frac{P_t}{P_{t,0}}$ is plotted in Fig. 42 for various indenter radius ranging from $R = 10\text{mm}$ to $R = 120\text{mm}$. Here, x_0 is the coordinate with the initial contact, $P_{n,0}$, and $P_{t,0}$ is the maximum normal and tangential tractions. It is important to note that, due to the coupling, the dimensionless plot of

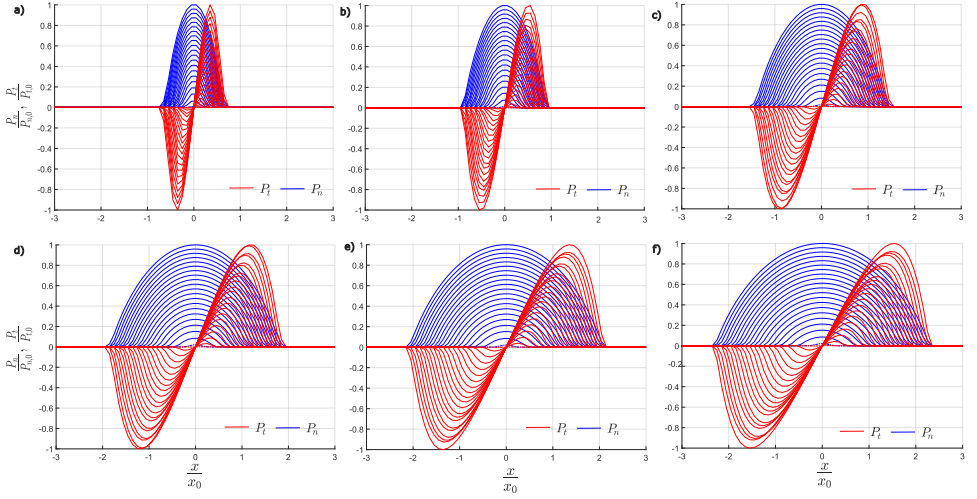


Figure 42: Dimensionless plots for the vertical (blue) and horizontal reactions (red) for indenter radius of, a) $R = 10\text{mm}$, b) $R = 20\text{mm}$, c) $R = 50\text{mm}$, d) $R = 80\text{mm}$, e) $R = 100\text{mm}$, and f) $R = 120\text{mm}$.

tangential tractions can also be multiplied with the friction co-efficient $\mu = 0.2$. In such a case, the positive slip of the tangential tractions coincides with the horizontal tractions, leading to dimensionless plots as in [75]. This study omitted the dimensionless plots considered friction coefficient μ for brevity. Moreover, the dimensionless plots show that horizontal and vertical tractions are strongly coupled with a dependency on the radius of the Furthermore, Fig. 42 can be said qualitatively equivalent to the work in [75], showing the ability of the model to reproduce. Moreover, as the radius increases, the contact area, consequently, the tractions evolve.

Furthermore, Fig. 43 and Fig. 44 show the contour plot for the displacement in x –, and y – direction for the $ts = 20, 40, 60, 80, 100$ sec as the time evolves. These figures shows the contour plots of the vertical and horizontal displacement fields showing the penetration of the cylinder. It can be observed that, initially, due to the indentation, the contact area is small, and as the displacement increases, the contact area increases, which is well represented by Fig. 44. Specifically, the horizontal tractions in Fig. 41 can be realized in the contour plot presented in Fig. 43.

Similarly, the contour plot for the x – directions shows both forward and backward slip, as elucidated in Fig. 41. Furthermore, the vertical traction in Fig 40 can

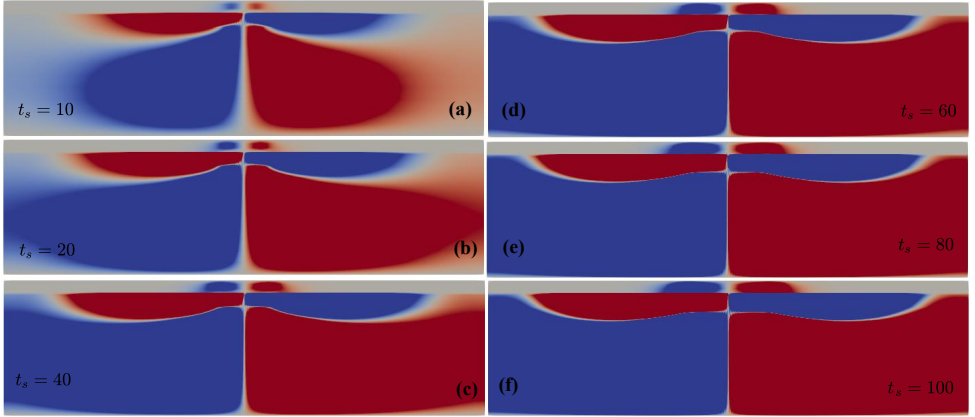


Figure 43: Contour plot of displacement in x-direction for $t_s = 20, 40, 60, 80, 100$ Sec

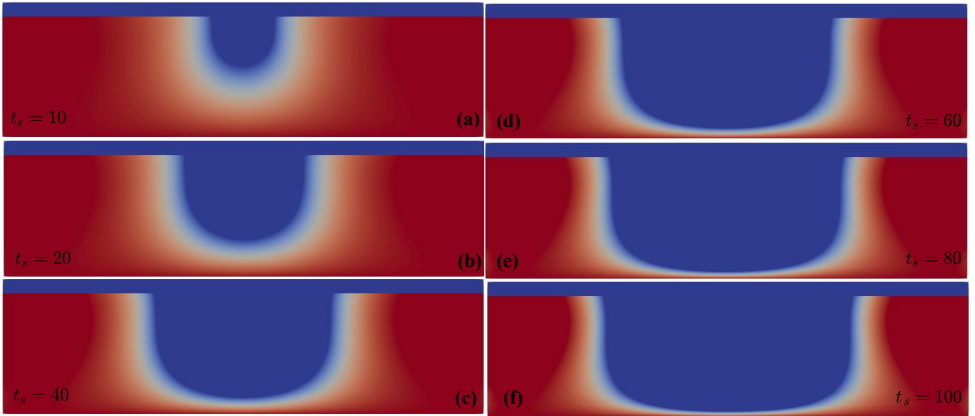


Figure 44: Contour plot of displacement in y-direction for $t_s = 20, 40, 60, 80, 100$ Sec

be realised in the contour plot presented in Fig. 44.

The wear rate is computed according to Archard's law of wear as a combination of the vertical and tangential tractions as in Eqn. (3.89). Fig. 45 (a) presents the wear rate profile at each position for $R = 100\text{mm}$. Since the material of the two contacting bodies is different, there is a strong coupling between horizontal and vertical traction. The slightly off centered plots at zero are due to the small applied horizontal loading. This offsets becomes zero as the radius of the indenter

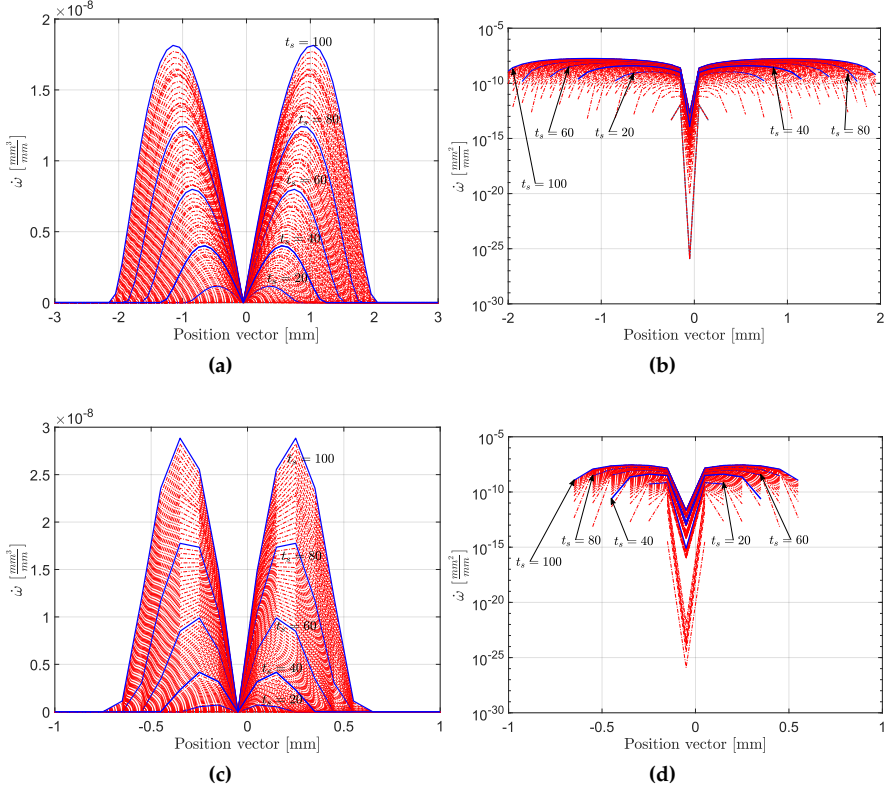


Figure 45: Wear rate for the cylindrical contact specimen with a) wear rate vs. position vector, b) wear rate and position vector in the logarithmic plot for contact radius of $R = 100\text{mm}$, whereas wear rate for the cylindrical contact specimen with c) wear rate vs. position vector, d) wear rate and position vector in the logarithmic plot for contact radius of $R = 10\text{mm}$.

increases, and is more visible when the radius of the indenter is very small. The Fig. 45 (a) shows that as the loading increases, the wear rate increases. Interestingly, the wear is induced in both the forward and backward slip positions, as seen in Fig 45 a). Furthermore, the wear rate closely follows the coupled tractions induced by the surface. Moreover, to further assess the wear characteristic, the wear rate is plotted in a logarithmic plot with respect to the position plotted in Fig. 45 (b). The logarithmic plot shows the wear rate more clearly in the scale at which it is feasible to see the evolution more sensibly. Consequently, it can be observed that, as time evolved, the wear spread out, with an expanding initial contact area.

To further elucidate the effects of the radius of the indenter on the wear rate, Fig. 45 (c) presents the wear rate with respect to the position vector. In contrast, Fig. 45 (d) presents the logarithmic wear rate at $R = 10\text{mm}$. It can be noticed that the wear rate is of the same order of magnitude in both the radius, with a slightly high wear rate for the smaller radius. Furthermore, wear spreads out less as the radius decreases, leading to a higher wear rate in line with the experimental observations.

Effect of indenter radius

Fig. 46 illustrates the effect of Variation of the indenter radius of the spherical indenter on the contact geometry. The radius of $R = 5, 10, 20, 50, 80, 100\text{mm}$ and $R = 120\text{mm}$ is used. Fig. 46 (a) presents the normal tractions at each position, whereas Fig. 46 (c) presents the tangential tractions at each position of the interface. Furthermore, Fig. 46 (b) and Fig. 46 (d) presents the corresponding dimensionless plots between $\frac{x}{x_0}$ Vs. $\frac{P_i}{P_{i,0}}$ for the normal and tangential tractions respectively. Here x_0 is the total length of the interface, and $P_{i,0} = \max P_i$ for the final time step $t_s = 100\text{sec}$. It can be noticed that as the contact area changes, the amplitude of the normal and tangential tractions increases. Furthermore, vertical traction shows that the depth or contact pressure decreases as the contact area increases, reducing the vertical traction with increasing radius. Finally, Fig. 47 (b) presents the wear rate for the Variation of the indenter radius, whereas Fig. 46 (a) presents the normalized rate for each radius. It can also be observed that the wear rate is a linear combination of the tractions. Moreover, Notice that the wear rate is small due to the (a) small coefficient of wear and (b) low loading cycle. Wear accumulates under low- or high-cycle fatigue, leading to more pronounced wear.

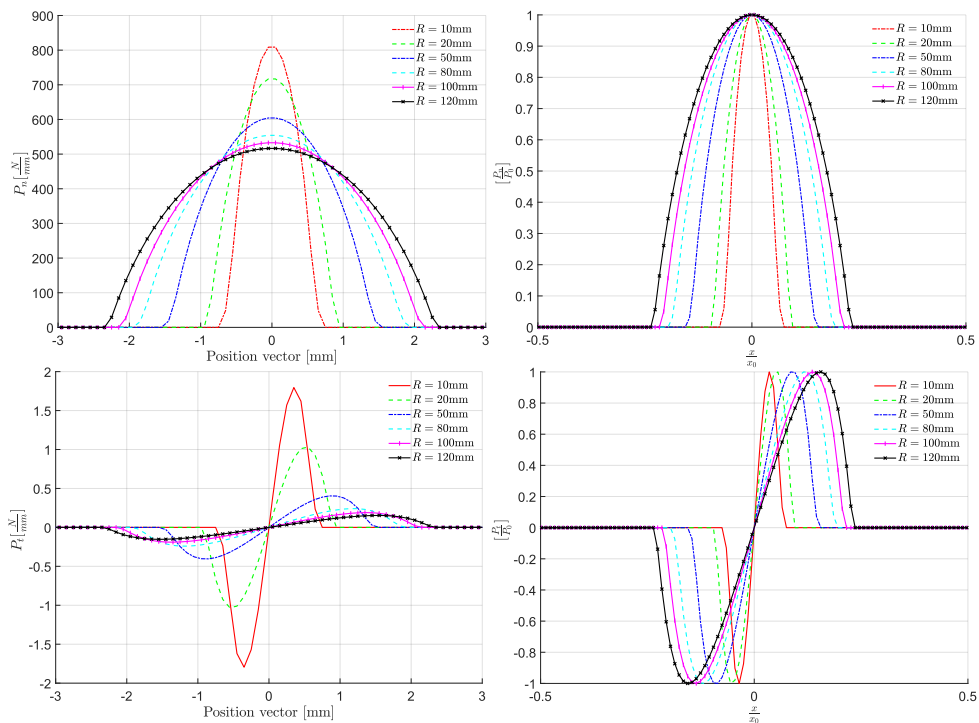


Figure 46: Traction for $R = 10, 20, 50, 80, 100, 120$ mm

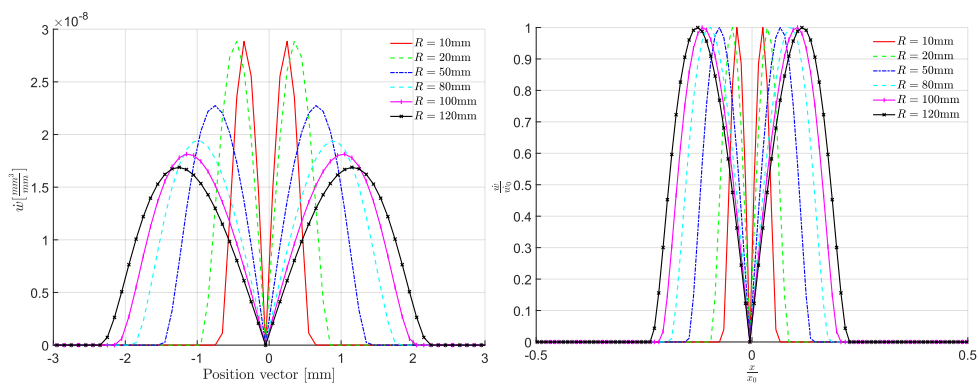


Figure 47: Wear Rate $R = 10, 20, 50, 80, 100, 120$ mm

Effect of wear coefficient

To accelerate the wear process, the coefficient of wear is increased. The wear coefficient quantifies the rate at which material wear occurs between two contacting surfaces under relative motion. The wear coefficient can change during the operation conditions, especially under the influence of lubrication. Within the context of the variational formulation, the wear coefficient is directly proportional to the wear rate, as in Eqn. (3.89). Hence, a wear rate ranging from $K = 10^{-7}$ to $K = 10^{-11}$ demonstrates that the tractions are displayed in logarithmic plots due to the large order of magnitude difference. Fig. 48 presets the wear rate in the logarithmic curve at each interface position. It can be seen that as the K increases, the wear is higher. As a result of this relationship, it is evident that if the K is decreased in the industrial setting, it leads to better design quality with reduced wear. Moreover, the wear coefficient is independent of the traction, leading to a constant dimensionless plot. Consequently, the dimensionless plots are omitted here.

Effect of friction coefficient

It is well known that friction coefficients also play a vital role in tribology. The roughness of the surface dramatically influences its value in Fig. 49, which presents the tangential tractions at each interface position. The friction coefficient μ varies from $\mu = 0.1$ to $\mu = 0.5$ when the non-linear displacement is applied in the horizontal direction, as in Fig. 39. It is clear that the value of μ increases, both the negative and positive slopes steadily increase and vice versa. As a consequence, the wear rate also changes.

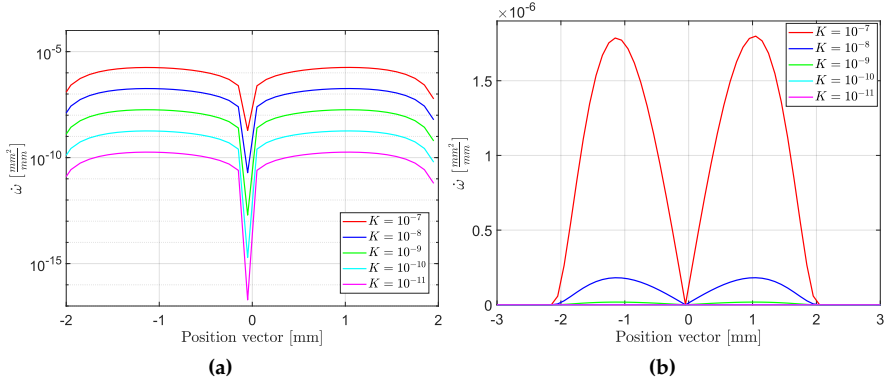


Figure 48: Wear Rate on different variations of wear coefficient on cylindrical indenter

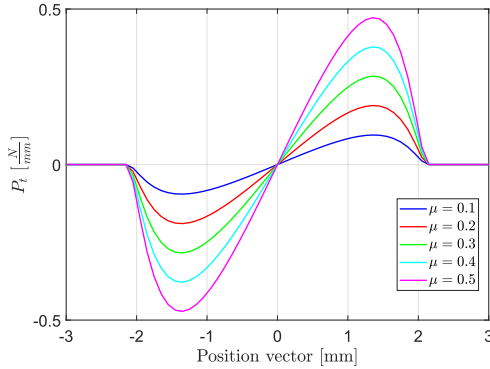


Figure 49: Horizontal Traction on different variations of coefficient of friction on cylindrical indenter

Effect of rate dependency

In this section, the rate dependency of the wear problem is shown. For this reason, the load is applied in different increments with different relaxation times. Specifically, the final time of the simulation $T_f = 5$ sec is kept constant for all the simulations, whereas the time increment dt and the number of steps t_s taken to reach the final time T_f is changed, such that $t_s \times dt = T_f$. Furthermore, $dt = \{0.01, 0.02, 0.03, 0.04, 0.05\}$ is taken. Consequently, the time increments lead to $dt = \{500, 250, 167, 125, 100\}$. Fig. 50a) and b) presents the normal and tangential trac-

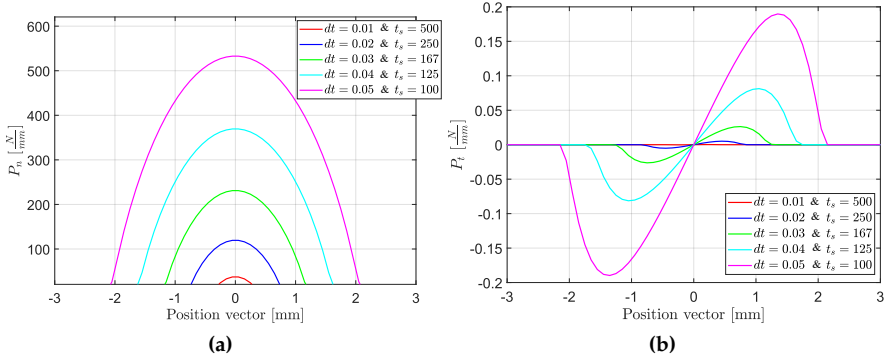


Figure 50: Time rate of change of tractions on cylindrical indenter

tions at each interface position related to the time rate change of the cylindrical indentation with the radius of $R = 100\text{mm}$. The coefficient of friction and the wear coefficient are kept constant with $\mu = 0.2$, $K = 10^{-9}$ respectively.

Fig. 51 presents each Variation's wear rate induced at each position in a logarithmic scale. It is easy to notice that the normal and vertical traction increases as the number of increments increases. Moreover, an increase in the wear rate is observed as the time steps increase. This leads to localized failure, causing more rapid wear at specific points along the interface. Furthermore, this could be because, as the contact pressure decreases with a higher time step, a more gradual interaction between the indenter and the surface is established, potentially leading to reduced wear rates over time. It can be seen in Fig. 51 that the blue colour profile with the lesser time increment reflects the higher time step at which the indenter makes contact when the vertical downward displacements are applied, resulting in lower contact pressure. This observation aligns with the anticipated behaviour based on the applied forces and material properties.

Furthermore, dimensionless plots for the Variation of the time rate changes for normal tractions are plotted in Fig. 52 (a), tangential tractions in Fig. 52 (b) and wear rate in Fig. 52 (c). The strong effects of the time rate dependency can be observed from these plots.

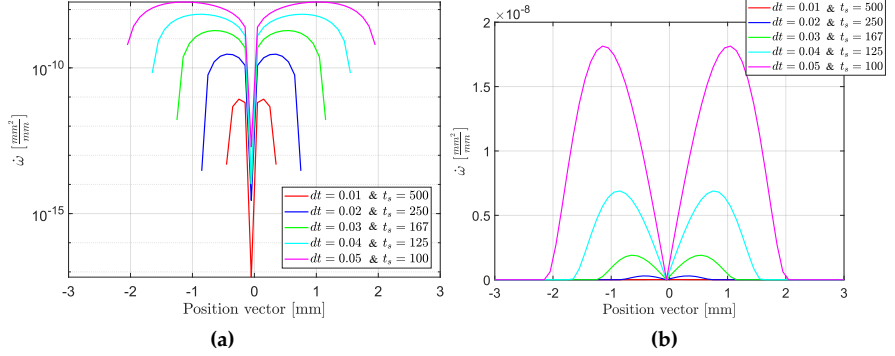


Figure 51: Time rate of change of wear on cylindrical indenter

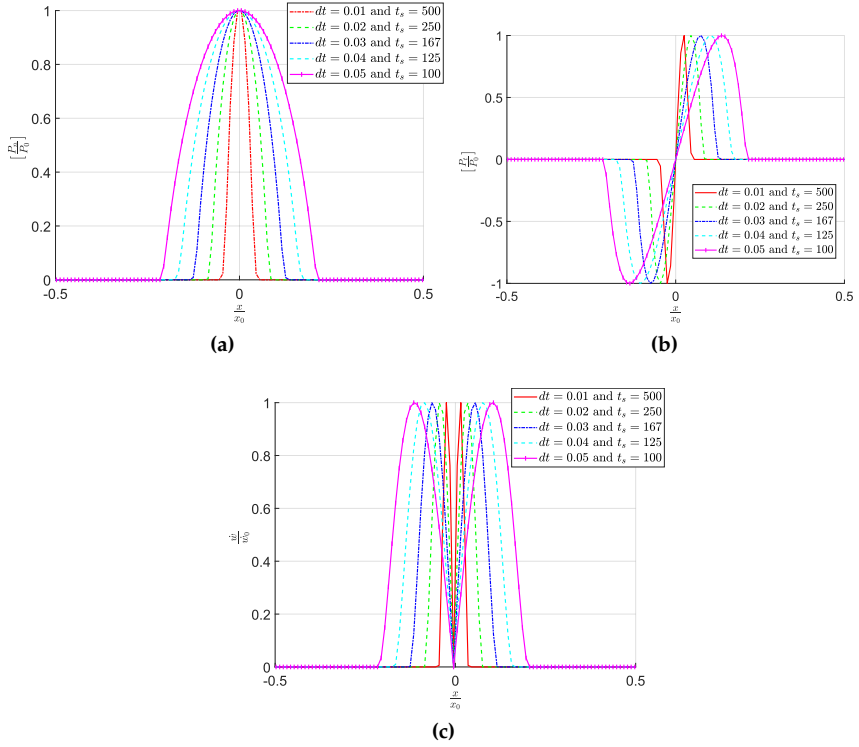


Figure 52: Dimensionless plots for the variation of time rate of change for a) vertical traction, b) horizontal traction and c) wear rate

4.3 Flat indenter

In this section, a flat, indented profile is evaluated. The indenter profile spans the whole interface, whose dimension is the same as shown in Fig. 37 (b). The indenter consists of the length $L = 10\text{mm}$ and thickness of $t = 0.5\text{mm}$. The material properties considered in this section are similar to those in Section 4.2 is used. The boundary conditions and the load histories remain the same. The wear coefficient is taken as $K = 10^{-9}$, and the coefficient of friction is taken as $\mu = 0.2$ unless specified.

The relative displacement between the contacting surfaces is taken as

$$h^* = 0 \quad (4.5)$$

consequently, separation equals the actual gaps computed from the displacement field.

Fig. 53 (a) presents the normal tractions at each interface position. It is easy to see that the flat surface penetrates the interface as the displacement load increases, creating a normal pressure. Until the $ts \approx 25$, the load is dominated by normal reactions, consequently leading to equal tractions across the positions. After the $ts > 25$, the normal tractions are strongly coupled with the tangential tractions, leading to unequal tractions from the middle and the edges. Furthermore, Fig. 53 (b) presents the tangential tractions at each position vector of the interface. It is easy to notice that there is no point of contact. Instead, the indenter comes in contact with the interface at all the points. As the tangential load is applied, the flat indenter puts a shearing load across the interface, loading it into mixed mode behaviour. Specifically, normal force induces Mode-I type behaviour, whereas tangential tractions introduce Mode-II. Consequently, the tractions at the centre of the interface are almost zero. But at the edges of the interface, the tractions are highest. In simple words, there exists a point in the interface where there are no tangential tractions, and at the edges of the interface, maximum tractions are observed. These are well reflected in Fig 53 (b). Fig. 53 (c) shows the dimensionless plots between the normalized vector $\frac{x}{x_0}$ and the normalized. Fig. 53 (c) shows that, due to the influence of the tangential tractions, the normal tractions at the boundaries are unequal compared to the initial contact pressure. Moreover, the dimensionless plot also presents a strong coupling between the tractions.

Fig. 54 presents the wear evolution in the interface due to the flat indenter. Specifically, Fig. 54 (b) presents the wear rate at each position vector along the

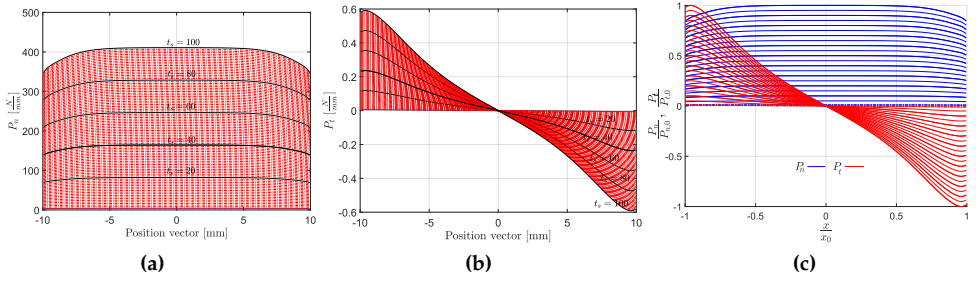


Figure 53: a) Vertical traction on flat indenter b) Horizontal traction on flat indenter c) Dimensionless plot

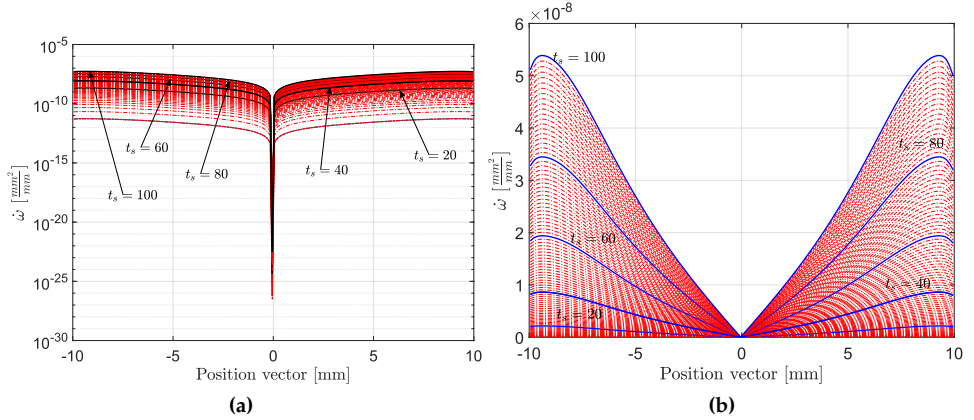


Figure 54: Wear Rate at flat indenter

interface, whereas Fig. 54 (b) presents the wear rate in the logarithmic plot. In line with the discussion, the wear rate at the edges is more significant than that at the middle of the interface. Moreover, as time evolves, the tangential tractions dominate the wear rate.

To accelerate the wear, the coefficient of wear is increased between $K = 10^{-7}$ to $K = 10^{-11}$, and the corresponding wear rate is presented in Fig. 55. Due to the varied order and magnitude of the Variation, a logarithmic wear rate is given. As expected, the coefficient of wear is found to be linearly proportional to the wear rate.

The roughness of the indenter is changed to access the effects of the various

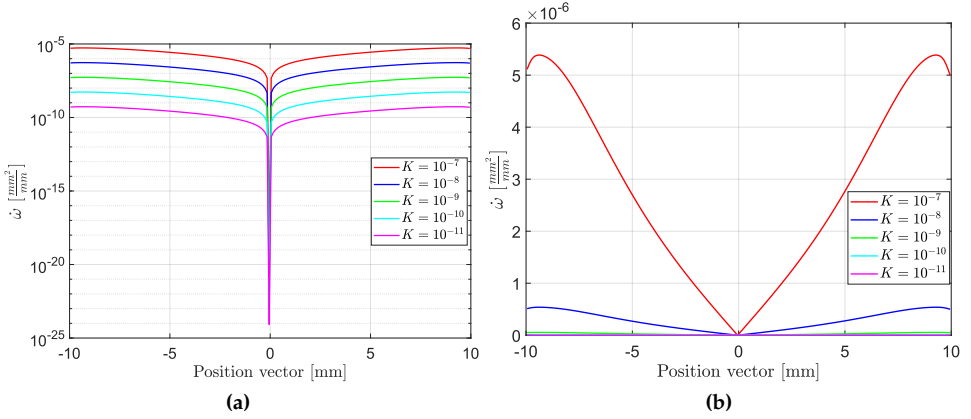


Figure 55: Wear Rate on different variations of wear coefficient on flat indenter

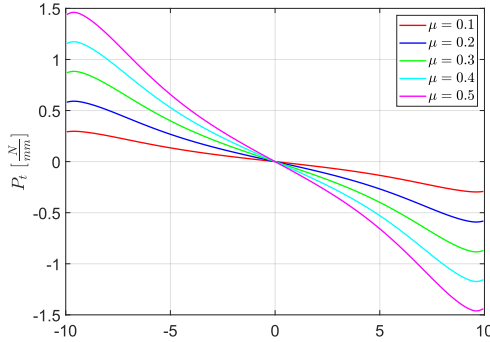


Figure 56: Horizontal traction on different variations of coefficient of friction on flat indenter

frictional constant $\mu = 0.1$ to $\mu = 0.5$. It can be noticed in Fig. 56 that as the friction coefficient increases, the tangential tractions increase; consequently, the wear rate increases. Furthermore, naturally, when the friction increases, the tractions at the edges increase, as shown in Fig. 56.

4.3.1 WM indenter

Introduction

A complex fractal profile is considered in this section to test realistic roughness profiles stemming from an engineering standpoint. The effectiveness of the proposal approach is evident from the complex shapes utilized in the section. Specifically, a fractal profile based on the Weierstrass-Mandelbrot function is used to create the complex surface of many harmonics. Even though many other functions can be utilized in the proposed framework to generate and assimilate the elevation produced by the complex surface, the WM function offers unique challenges regarding the numerical implementation. Furthermore, its fractal nature demands high-precision computation. Hence, the WM function is chosen to showcase the robustness and versatility of the presented computational framework in a high-fidelity framework. The elevation field given by the rough profile can be generated as a fractal function with harmonic given by

$$h^* = g_0 \sum_{n_w=0}^{\infty} \gamma^{(D-2)n_w} \cos\left(2\pi \frac{\gamma^{n_w} x}{\lambda_0}\right), \quad (4.6)$$

where g_0 is the initial gaps, n_w is the harmonics. Furthermore, λ_0 is the wavelength of the largest scale roughness, D is the fractal dimension, and γ is a parameter defining the inverse ratio between successive wavelengths in the profile. The cosine function is summed over the n_w to create a superposition of the n_w sinusoidal waved of the wavelength $\lambda_{n_w} = \frac{\lambda_0}{\gamma^{n_w}}$, and the amplitude $z_{n_w} = z_0 \gamma^{(D-2)n_w}$, with $\gamma > 1$. The fractal dimension can be computed as $1 \leq D \leq 2$.

The geometric description is shown in Fig 37, with a flat lower edge and the top edge is embedded with the rough WM function. As a balance between computational efficiency and the complexity of the WM profile, the first four harmonics of the WM functions are chosen, i.e. $n_w = 1, 2, 3, 4$. The height field aligns with a typical discontinuity in the initial undeformed state. To capture the geometric features of the profile, a mesh size of at least 20 elements is used to simulate each wavelength. Therefore, the number of interface finite elements used depends on the number of terms in the Weierstrass series. Specifically, for $n_w = 1$, a mesh size of $h = 20$ elements are used, for $n_w = 2$, $h = 80$, for $n_w = 3$, $h = 320$, and finally for $n_w = 4$, a mesh size of $h = 1280$ elements are used. The presented discretization has enough elements to capture the wear profile, stress and strain states. Due to the fixed lower plate, initial values of $g_0 = 0.006$, $D = 1.25$, and $\gamma_0 = 0.6$ are chosen for

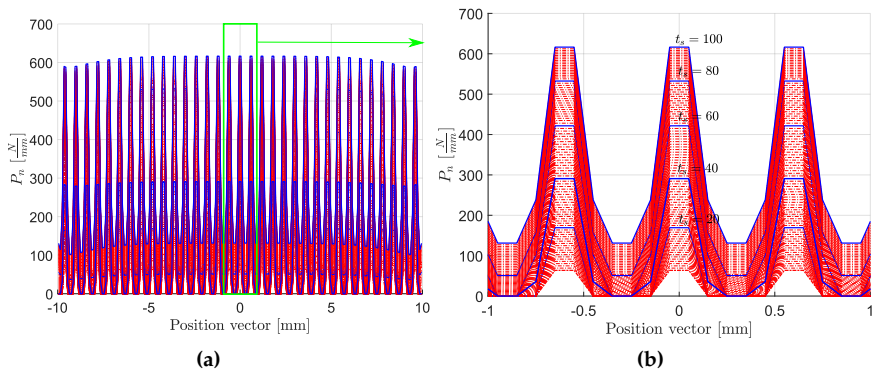


Figure 57: a) Vertical traction of the embedded rough profile of the specimen, b) zoom in view

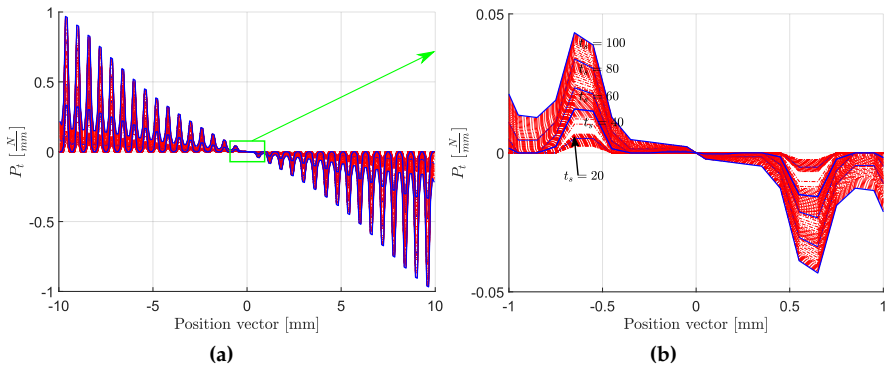


Figure 58: a) Horizontal traction of the embedded rough profile of the specimen, b) zoom in view

the initial profile.

Fig 57a) presents the vertical traction for the embedded rough profile with WM function for third harmonics $n_w = 3$. Due to the many harmonics, the sinusoidal curve hinders the evolution of the tractions. Hence, a focused-in view of the vertical traction between $x = [-1, 1]$ is presented in Fig. 57 (b). The evolution of the vertical tractions can be seen in Fig 57b). Furthermore, it is easy to notice that, initially, the points of contact and, subsequently, the area of the contact change as time evolves. Due to the coupled loading history, the normal tractions initially increase faster and reach a constant linear evolution.

Fig. 58 (a) presents the tangential tractions for the rough profile with WM function for the third harmonics $n_w = 3$. The impact of the WM indenter on the surface can be seen as a point of contact. Due to the initial contact, the area of the indentation is small. Subsequently, the tangential tractions at the leading edge increase the contact area and reduce as the trailing edge. The reversal in the tractions can be seen in Fig. 58 (a) can be seen. Furthermore, Fig. 58 (b) presents the zoomed-in view of the tangential traction between $x = [-1, 1]$. The tractions' localized tangential tractions' reversing can be seen clearly as the traction evolves, as in Fig. 58 (b).

Subsequently, the evolution of the wear profiles in the WM functioned in Fig. 59. The coefficient of friction is $\mu = 0.2$, and the coefficient of wear is $K = 10^{-8}$. Fig 59a) presents the wear at each position of the interface, whereas Fig. 59 (b) presents the wear at $x = [-1, 1]$ to present a zoomed-in view. Furthermore, the figures also present the evolution of the wear. It's interesting to note that, due to the coupled loading, when only vertical force is applied, the wear rate increases slowly, followed by a big change after applying the tangential load. Moreover, Fig. 59 (c) presents the wear rate in the logarithmic plot, whose zoomed-in view can be seen in Fig. 59 (d). It is easy to notice that the wear rate is significantly higher than the other parts at the point of the first contact. In other words, the trough of the WM functions produces a higher wear rate than the WM function's crest.

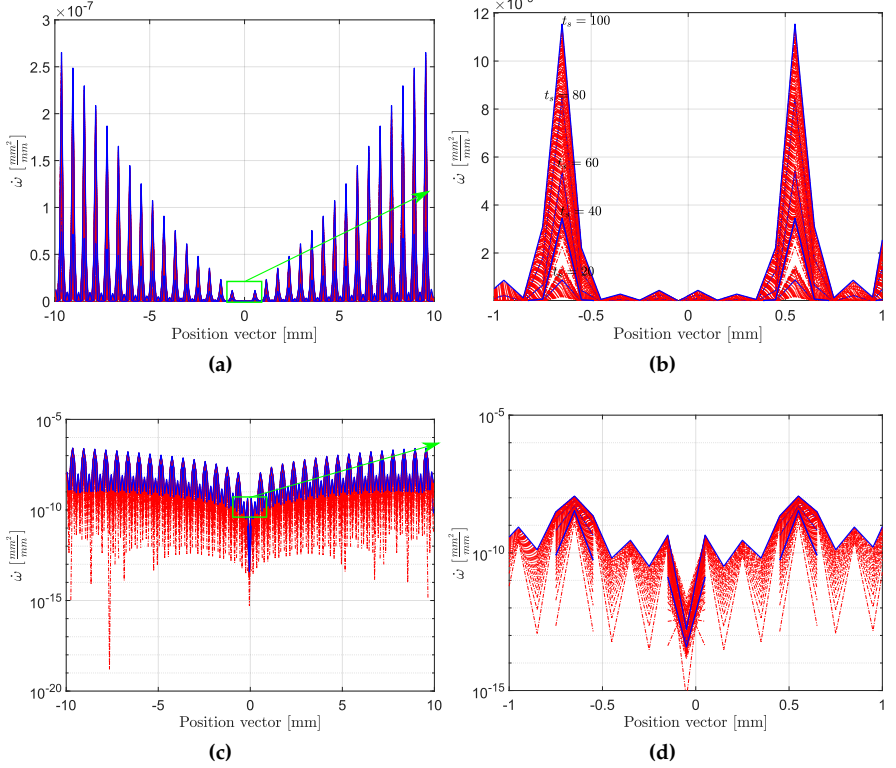


Figure 59: Wear rate for the embedded rough contact, a) wear rate vs. position vector, b) zoom-in view, c) wear rate vs. position vector in logarithmic plot and d) zoom-in view of the logarithmic plot

Effect of number of Harmonics

This roughness uses a profile of varying harmonics in this section to showcase the proposed model's effective predictive capability. Fig. 60 presents the contour plots for the Variation of the harmonics. In total, four different harmonics with $n_w = 1, 2, 3, 4$ as in Eqn. 4.6 is considered. Consequently, a displacement contour in the x-direction is presented in Fig. 60 (a). It is easily observed that the slip conditions corresponding to the tangential tractions can be seen. Furthermore, Fig. 60 (b) presents the displacement contour in the y-y-direction. The point of the contact shows that, as the number of harmonics increases, the displacement profile adjusts accordingly, leading to a harmonic displacement. Consequently, the principal stresses are presented in Fig. 60 (c) for the direct stress σ_{yy} . The principle stress also indicated the strong presence of the turfs and crests in the WM function. Furthermore, the stress is localized turfs, and the crests are stress-free. The Contour plots also present the transfer of forces from the top layer to the bottom by the presence of the interface.

To comprehensively understand the effects of the rough profile, the normal tractions along the interface are presented in Fig. 61 (a). To elucidate the repeated nature of the harmonics, Fig. 61 (b) presents the normal tractions for the position between $x = [-2, 2]$. As the number of harmonics increases, the point of contact also increases. Consequently, higher normal tractions are seen for each increase in the harmonics. Notice that the sinusoidal functions presented here are not entirely sinusoidal but a reconstruction of the sinusoidal functions with finite linear elements. Consequently, the smoothness of the functions at the minima or the maxima is lost, leading to the tractions as in Fig. 61.

Similarly, the tangential tractions for each position vector of the interface for the Variation of the number of harmonics are presented in Fig. 62 (a). Furthermore, tangential tractions for the position vectors $x = [-2, 2]$ are presented in the Fig. 62 (b) for a concise understanding.

The wear rate for the rough profiles for the WM functions is presented in Fig. 63. The effect of variation of n_w in the wear rate shows the reduction of contact area as n_w increases, which develops the wear by the evolution of the stick and slip area. In addition, the change in the contact area and the wear rate is also decreasing, as seen in Fig. 63. The logarithmic plot Fig. 63 (c) and (d) gives a more precise idea of wear rate w.r.t the change in n_w .

Dimensionless plots for each harmonic are plotted to comprehend the roughness profile further. Specifically, the normalised position vector are plotted against

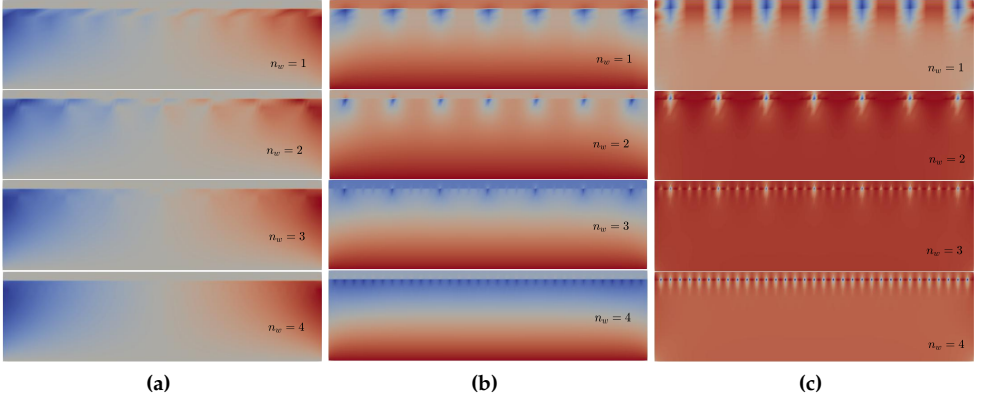


Figure 60: Contour plots of the Variation of n_w , a) displacement in the x-direction, b) displacement in the y-direction and c) principal stress, σ_{yy}

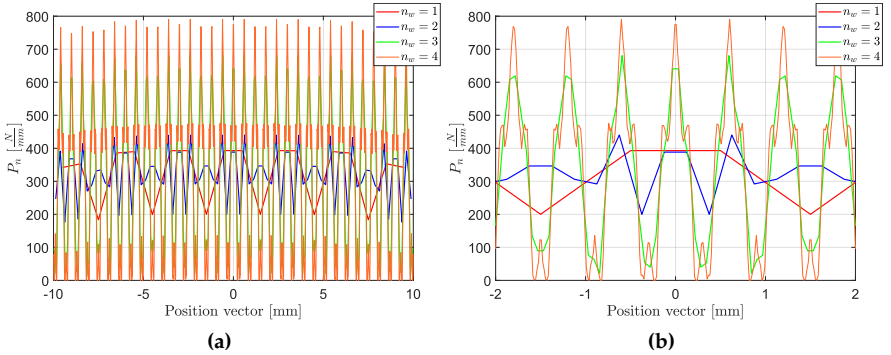


Figure 61: Variation of n_w a) vertical traction of the embedded rough profile of the specimen, b) the vertical traction along the interface for position vector between $x = [-2, 2]$.

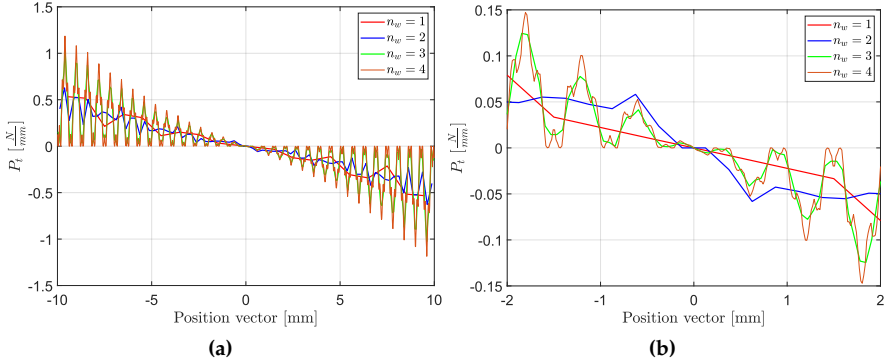


Figure 62: Variation of n_w a) horizontal traction of the embedded rough profile of the specimen, b) zoom in view

$\frac{P_n}{P_{n,0}}, \frac{P_t}{P_{t,0}}$ are plotted for $n_w = 1, 2, 3, 4$. Fig. 64 (a) presents the dimensionless plot for the $n_w = 1$. This plot shows the evaluation of the normal and tangential tractions as time evolves. Interestingly, the coupled tangential tractions remain dormant until the tangential loads are applied. In contrast, as soon as the tangential load is applied, the tangential tractions increase significantly. This is observed in all the cases. Furthermore, Fig. 64 (b) presents the dimensionless plot for $n_w = 2$. Notice that the second harmonic function possesses greater crests and turfs, consequently leading to a higher contact area. Fig. 64 (c) and (d) present the dimensionless plot for $n_w = 3$ and $n_w = 4$, respectively. Due to the significant harmonics, only the maximum tractions at $ts = 100$ are presented, whose evolution is omitted here for brevity.

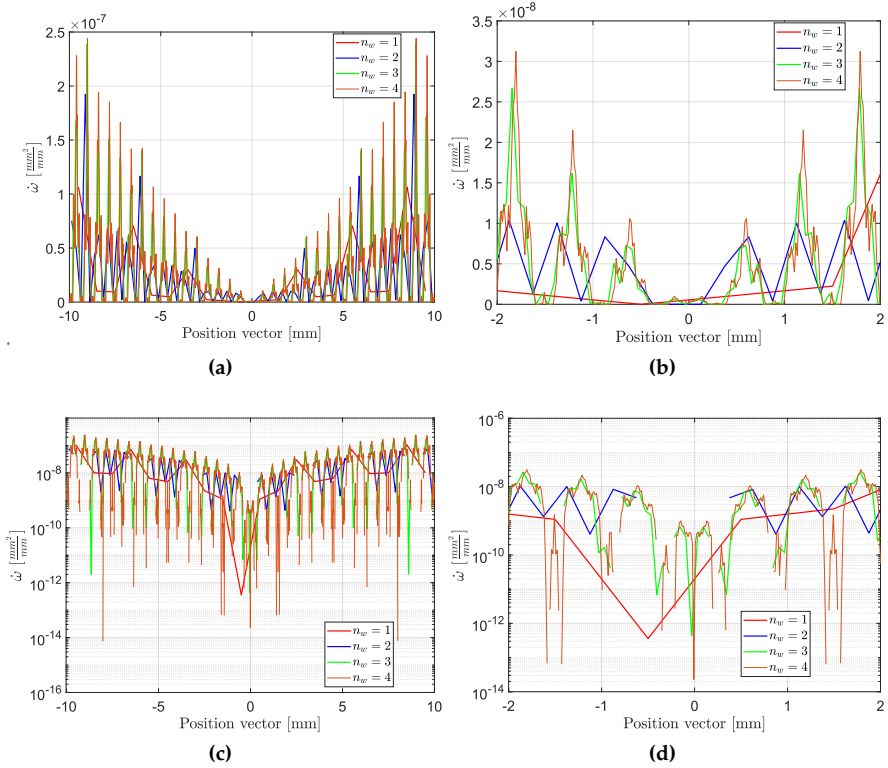


Figure 63: Variation of n_w for the embedded rough contact a) wear rate vs. position vector, b) zoom-in view, c) wear rate vs. position vector in logarithmic plot and, d) zoom-in view of the logarithmic plot

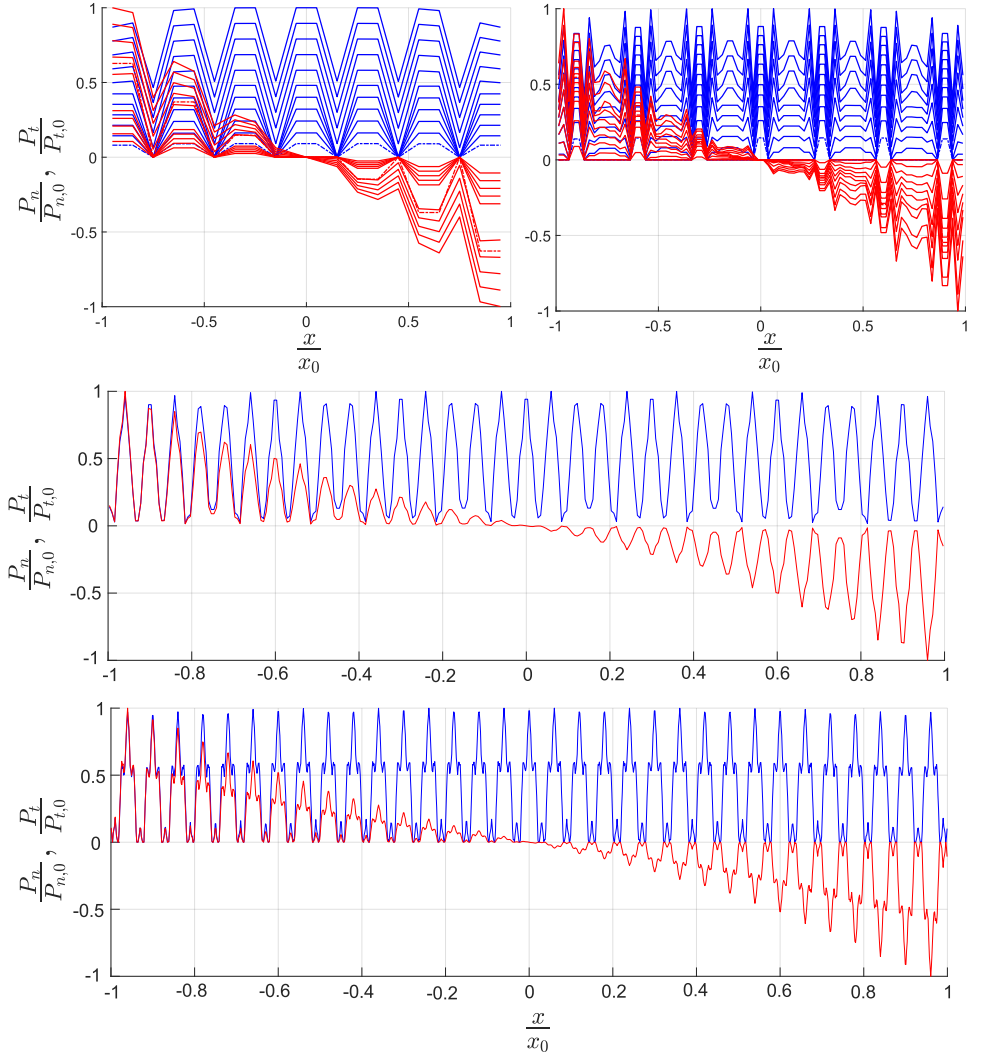


Figure 64: Dimensionless plot for $n_w = 1$, $n_w = 2$, $n_w = 3$, and $n_w = 4$. Red lines present the tangential tractions, whereas blue lines present the normal tractions

Chapter 5

Conclusion and Future Development

The present formulation in the thesis solved the contact problems between rough and complex profiles and surfaces. Chapter 2 introduces polycrystalline diamond material for testing. The experiment was used with a Tribotest machine to exploit PCD at different loadings under sliding motion. The results presented in section 2.3 of varying surface finishes of grades 600 and 820 of PCD show the capabilities of PCD. The surface finish and micro-structural images were presented and briefly discussed after and before the experiment.

Chapter 3 introduces a comprehensive 2D formulation of an interface element originally used in non-linear fracture mechanics. The process begins with the strong equilibrium form and derives the corresponding weak form, ultimately arriving at a non-linear system of equations suitable for integration into conventional FEM software (FEAP). An extension of the interface element is presented, based on the framework initially proposed in [45] and subsequently expanded in [75], enhancing its capabilities to address rough contact issues. Utilizing the previous work, a new framework for predicting wear is introduced, improving the formulation's capabilities.

Chapter 4 tests the proposed model using many benchmark problems, mainly using three indenter profiles. Specifically, the indenter with spherical, flat and the WM function is used to present the model's capabilities. Furthermore, dimensionless analysis is used to analyse the wear profiles comprehensively. The model's capabilities are tested by considering various profiles and parameters. Finally, the

proposed model shows a good correlation with the previous results regarding the contact problem, followed by the successful prediction of the wear profile according to the physics.

5.1 Future Developments

Several key potential research areas can be identified along this research line. Some are natural extensions of the proposed work in this thesis, and others stem from a long-term perspective. The future developments can be broadly classified as (i) Extension to Hilti, (ii) Experimental, (iii) numerical approximations, and (iv) multi physics problems.

5.1.1 Extension to Hilti

The proposed model serves as the initial stage of an ongoing comprehensive development. Specifically, the model describes the wear profile under half-slip conditions with static loading. Our next priority is to expand this to full slip conditions, followed by combined horizontal and vertical loading. The model will also be extended to incorporate roughness in both the cutting and substrate profiles through statistical analysis. Additionally, we will include a micro-mechanical analysis to depict material behaviour under full slip conditions accurately. Furthermore, the model will be expanded to encompass fatigue loading, allowing us to estimate the lifetime of the PCD samples. Hilti-Schaan is also keen on understanding the fracture behaviour of these materials under static and fatigue loading. Finally, the full slip fatigue model will be further developed to include fracture using Phase-field methods. As we aim for the long-term efficiency of the mathematical model, we propose variational methods for wear as a starting point in this thesis.

5.1.2 Experimental Wear

Chapter 2 will provide detailed insights into the performance of PCD material in dry conditions and the results obtained from the sliding test. It was noted that temperature variations or thermal imaging equipment were not accounted for in the experimental investigations. Monitoring temperature changes on the samples during the experiment by employing thermocouples is imperative for a comprehensive understanding of the influence of temperature on wear. The interplay of tempera-

ture and friction is pivotal in assessing wear rate. Consequently, future experiments will be tailored to investigate the role of temperature in wear evaluation.

The examination of wear tracks on PCD samples post-test has revealed notable disparities between polished and unpolished surfaces regarding their roughness. This analysis of wear tracks has yielded crucial insights into the impact of surface treatment on wear resistance. It has been observed that polished samples exhibit less material loss compared to their unpolished counterparts, indicating the critical role of surface smoothness in reducing friction and wear. Furthermore, a comprehensive assessment of the roughness parameters has confirmed that lower roughness values in polished samples are linked to reduced wear rates. A smooth surface finish mitigates surface interactions and enhances the longevity of PCD materials under operational stress. These findings underscore the significance of surface preparation in applications where wear is critical, emphasizing the need for rigorous quality control in the manufacturing process to ensure optimal performance characteristics.

In chapter 2, the PCD material exhibited high wear resistance with a lower friction coefficient in the sliding wear test due to the diamond layer. To further understand the impact resistance of the samples, future experiments will be designed to assess the sample's ability to absorb energy resulting from an impact without failure. Additionally, it is essential to analyze the micro-structural characteristics of the PCD samples post-impact to elucidate the mechanisms that enable the diamond layer to withstand stress and recover from deformation. These analyses will incorporate advanced imaging techniques, such as scanning electron microscopy (SEM) and X-ray diffraction (XRD), to gain insight into the development of novel fracture patterns and potential changes in the crystalline structure of the diamond layer.

Moreover, the conducted test was confined to polycrystalline materials of grades 600 and 820. Additionally, future tests will include other PCD grades and hard materials to examine the relationship between wear and mechanical properties, such as hardness and elasticity, since these properties significantly influence wear resistance.

Furthermore, research will be conducted on the impact of surface treatments and coatings on wear performance, such as polycrystalline diamond samples with a high-resistance diamond coating. Therefore, various other surface modifications, including different hard coatings or surface hardening techniques, can evaluate wear behaviour under consistent testing conditions. This comparative study will

provide insights into the effectiveness of these treatments in improving wear resistance and facilitating the development of materials with superior performance in challenging applications.

5.1.3 Numerical Approximations

The presented numerical approximation poses several advantages and disadvantages in the computation of the wear profile. The benefits include seamless integration with the material models and various indenter profiles. However, its mode can only calculate the wear for very small loadings. The natural extension of the model is to include repeated loading cycles. This can be achieved by incorporating the driving force based on the history variable and driving the wear profile based on the number of cycles. Furthermore, cycle-jumping techniques based on the history variable can be utilized to reduce computational expenses. This model can provide a real-time wear performance in various material models.

Another drawback of the proposed model revolves around using the real-time roughness profile. The roughness profile from real-time can be captured using profilometer experiments, and the roughness of the surface can be fed into the proposed model to describe the wear profile accurately. This can be added with no or few modifications to the proposed model. Furthermore, combining the rough profile from the profilometer with the capability of cycling loading can be of industrial significance.

Furthermore, wear such as fretting wear and abrasive wear can be added to the proposed model. In the industrial setting, wear is often followed by a fracture process. It is essential to stop the micro-cracks formed during the wear to nucleate. Consequently, combining fracture mechanics as a consequence of cyclic loading would benefit the industrial application. From the perspective of the proposed model, this can be achieved using two different methods. (I) The interface is modelled as in this thesis, and the bulk is modelled using fracture mechanics techniques, such as the phase field method to fracture. (II) The interface can be modelled as a combination of the wear and the phase field capable of nucleation, and the bulk is modelled with the phase field capable of propagation. Such models can accurately describe the wear process in industrial settings.

5.1.4 Multi-Physics Wear

As mentioned in the experimental wear, temperature plays a vital role. Experimental results show that the temperature changes the surface roughness and wear profile. Moreover, as the temperature changes, the construction associated with the material also changes, consequently changing the wear. The lubrication is primarily used to reduce the effects of temperature on the wear, which can be readily seen in processes such as cutting and drilling, to name a few. The coupled mechanical temperature becomes highly important in understanding wear within this context. From the perspective of this thesis, an extension of the proposal to the coupled temperature-displacement problem would be helpful. Furthermore, the effects of chemical processes and hardening rules would benefit the industry. The coupled multi-physics analysis, such as moisture, hygro-mechanical, and chemo-thermo-mechanical analysis of the wear, can provide an overall picture. Furthermore, from the tribological perspective, the effects of convection and radiation heat flow in the process, such as cutting and drilling wear, can be critical to the industries.

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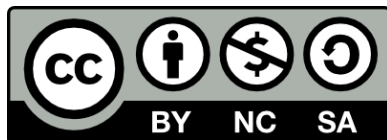
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