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Numerical Modelling of Soft Blasting on Polymeric Materials and Validation With Experimental Activities

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Abstract

Soft-blasting as a surface treatment, is utilized in operations where there is need to alter the surface of a substrate by plastically deforming it with shot media impact. It is also applied to modify surface morphology of polymeric substrates. These morphology modifications can have a variety of motivations like the enhancement of the wettability, which is followed by the phenomenon that a surface with induced roughness exhibits a modified state of wettability depending on the original state of wettability and the level of surface modification. For the concept of this thesis, a numerical model of soft-blasting is created and validated with experimental findings. The created model is validated over several impacting sequences of Alumina shot powder onto Polycarbonate (PC) substrate material. Model considers parameters of the soft-blasting machine equipment as well as substrate and shot media material properties. For a process like soft-blasting, shot media irregularity is an aspect to consider. The model takes into account the randomness of impacting sequence based on shot particles geometrical properties and shape fractions. The model, with its being a valid interface for soft-blasting simulation, stands also as a reference for future studies where surface-related properties will be under examination after surface treatments such as soft-blasting.

Keywords: Polymers, Surface treatment, Soft-blasting, Finite element analysis, Numerical model.

Sommario

La sabbiatura come trattamento superficiale, viene utilizzata nelle operazioni in cui è necessario alterare la superficie di un supporto deformandolo plasticamente con l'impatto del supporto di sabbiatura. Viene anche applicato per modificare la morfologia superficiale dei substrati polimerici. Queste modificazioni morfologiche possono avere diverse motivazioni come il miglioramento della bagnabilità, a cui fa seguito il fenomeno per cui una superficie con rugosità indotta mostra uno stato di bagnabilità modificato a seconda dello stato di bagnabilità originario e del livello di modificazione superficiale. Concetto di questa tesi, un modello numerico di sabbiatura viene creato e validato con risultati sperimentali. Il modello creato viene convalidato su diverse sequenze d'impatto di polvere di allumina su materiale di substrato in policarbonato (PC). Il modello considera i parametri delle attrezzature della macchina per sabbiatura morbida, nonché le proprietà del materiale del supporto e del supporto di sabbiatura. Per un processo come la sabbiatura, l'irregolarità del materiale di sabbiatura è un aspetto da considerare. Il modello tiene conto della casualità della sequenza di impatto in base alle proprietà geometriche delle particelle e alle frazioni di forma. Il modello, essendo una valida interfaccia per la simulazione della sabbiatura, rappresenta anche un riferimento per studi futuri in cui saranno in esame dopo trattamenti superficiali come la sabbiatura.

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Chapter 1

Introduction

This Master of Science Thesis study aims to develop a numerical model of soft-blasting operation and validating it with experiment.

Soft-blasting is technically similar process to shot-peening where particles impact on substrate surfaces with high velocities. This operation is mainly done in order to achieve enhanced fatigue performances of the parts as it creates residual stresses on the zone [1].

Another benefit of using this process-family is one of the recent topics studied in the literature. Several articles demonstrate the roughness effect on wettability phenomenon of substrates. This effect is mainly evaluated with the increase in the water contact angle occurring in water interaction on substrate surface that has a given roughness. The wettability enhancement of a surface mainly depends on the initial wettability state and induced surface roughness. Shot peening-soft blasting process family is quite suitable for altering roughness on a surface.

Having its own set of parameters in soft-blasting, the need for obtaining a numerical model which can take material properties and machine parameters as inputs and roughness parameters as outputs can save a high amount of experimental duty and give the advantage of creating a data set of important parameters through complete process.

Combining these facts, this thesis study has the objective of creating a numerical model, completely simulating soft-blasting operation with all of the steps included and provide a model ready to include wettability phenomenon in the future studies.

1.1 Soft-Blasting

Soft-blasting, also known as sandblasting is a mechanical process in which a shot media (may be referred to as “sand” or “powder”) is impacting on a substrate surface (may be referred to as “target”) with given amount of acceleration on the particles to ensure occurrence of plastic deformation and thus creation of compressive residual stresses on the impact zone.

Main motivation behind applying soft-blasting is to remove unwanted elements (i.e. contaminants) from the surface. Besides, it can also be utilized as a pre-process for a surface-enhancing operation. It can be a prior operation to painting where paint can be applied with a better efficiency with an altered surface roughness [2].

Soft-blasting can be processed for the purpose of varying motivations. Not only for removing contaminants, but it can also be applied to induce roughness from an as-built surface or even make a surface reduce its roughness with regards to initial state. Roughness is a characteristic that effects many interaction-related concept of a part surface. Thus, controlling roughness and the related characteristics over soft-blasting operation has been a promising technology.

Figure 1.1 shows the surface morphology development of copper substrates under different durations of sandblasting operation. It can be noticed that roughness increases with the increase in the duration of sandblasting [3].

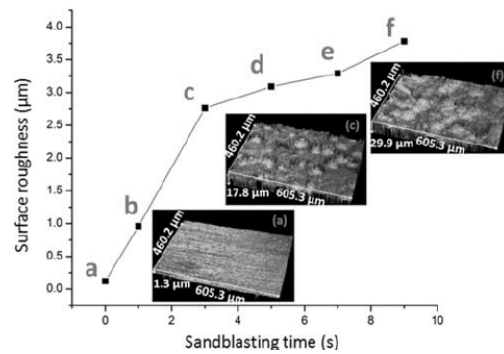


Figure 1.1: Surface roughness R_a vs. sandblasting time. (a), (c), and (f) are 3D surface images taken by profilometer showing the surface morphology of the samples sandblasted for 0 s, 3 s, and 9 s, respectively [3]

Soft-blasting and the effect of its application on the surface is studied under different disciplines. The process itself is clearly suitable for rust removal

from surfaces. With this point of view, Raykowski et al [4]. examines the utilization of stainless steel and glass spherical shot media in the blast-cleaning processes of gas turbine components. The motivation in that study is to evaluate the most effective parameters in the blasting process and determine a working condition that successfully removes deposit without deforming the substrate. The study led to the result that using a softer shot material (stainless steel in the study) than the substrate fulfilled the goal of the study and removed the deposits from the gas turbine component without deforming it.

Surface modification in the utilization of sandblasting is also examined in the literature. Chintapalli et al. [5] utilizes sandblasting in the dental restorations sector. It is stated that tetragonal zirconia doped with 3 mol % of yttria (3Y-TZP) is used in dental restorations because of its higher strength with regards to different ceramic oxides. Yet, tetragonal-monoclinic (t-m) transformation which tends to occur in front of propagation crack is a critical information for the long term performance of the material. This transformation occurs in accordance with application of sandblasting on the surface of 3Y-TZP. The study focuses on sandblasting effect on 3Y-TZP application in dental restorations.

In another paper by Chintapalli et al. [6], sandblasting is again used to process on 3Y-TZP. The motivation is to examine the effect of different sandblasting conditions such as different particle sizes, pressures and impacting angle on the mechanical properties of the substrate.

The abrasive media used to impact the substrate can be of various types including; sand, shot (in metal applications), glass, coconut shells and even dry ice [2]. Yet, the type of utilized impacting media has been an issue that led the way for the development of the technology throughout the history.

Sandblasting application is a process that is already present in the nature. Wind blowing over rocks and smoothing them with sand over the years is the principle behind the technology. Utilizing the same process in a faster way was the key element in the introduction of the process into scientific era. Benjamin Tilghman built a machine in 1870 with the purpose of removing paint and rust from the material surface with this nature-born erosion mind set [7] . The introduction of compressed air into process is done by Thomas Pangborn in 1904.

Yet, the process is regarded as unsafe as the unprotected utilization of sandblasting led the disease called silicosis in the lungs of workers which is

due to the accumulation of silica in the lungs as silica sand is used in the sandblasting process. To overcome this problem, a great milestone in the technology is achieved in 1918 with the introduction of enclosures into the machinery with a clear viewing screen letting the worker see the operation zone without a problem [7].

The equipment utilized in soft-blasting has different types. These different types mainly differ based on mobility requirements and the size of the part that will be soft-blasted. 3 major types are as the following:

Portable blast equipment: These devices include air compressors and blast pots that are pressurized with high pressure air obtained from air compressor. The most important advantage of this type is its mobility.

Blast cabinet: One of the most used and commercial types. It ensures the recycling of the abrasive as it has a conical shaped sand collector. In a zone that is enclosed but still possible to be viewed from a viewing window, remains the blasting system. A dust collection system also contributes to the functioning of the machine.

Blast room: Big size version of blast cabinet. The size varies depending on the scale of the processed part.

The representative figures of the equipment types can be seen in Figure 1.2.

The technical prospect of the methodology is quite similar to shot-peening with having the main exception as the motivation for the process. In shot-peening applications main motivation is to enhance life-cycle of the component by using its plasticity. Even if plastic deformation takes place with same functionality, the motivation in soft-blasting is to prepare a component for a future process or develop one of the characteristics of the component under a phenomenon in prospective works. Wettability phenomenon can be considered here as an example. The main motivation in using soft-blasting in this thesis is to alter surface roughness in favor of wettability for future studies. From the material point of view, it can be stated that, in shot-peening applications metals are mostly utilized. However in soft-blasting applications, different material families can also be used like Polymers as substrate and Alumina as shot media.



Figure 1.2: Blasting machine types

Figure 1.3 shows the principle of shot peening-soft blasting process family. Accelerated shot particles impact onto the substrate surface with high velocity and create a dimple as it forms a plastic deformation on the zone out of impacting particle kinetic energy.

The main factors of soft-blasting are the machine parameters that mainly effect the operation quality within the machinery. These machine parameters are:

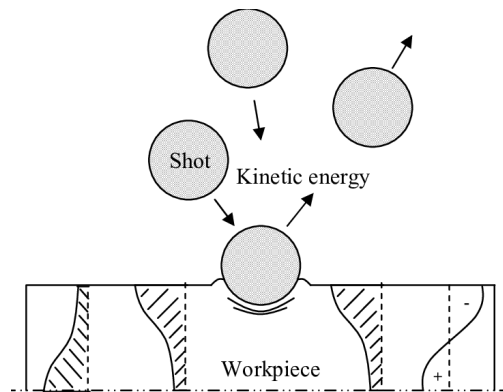


Figure 1.3: Principle of shot peening process [11]

- Air Pressure
- Stand-off Distance (SoD)
- Impact Time

The resulting surface morphology surely depends also on the substrate and shot materials and their properties. As the plastic deformation will be induced by the kinetic energy of the impacting particle, impact velocity of the shot is a very important factor. Impact velocity is highly influenced by Air Pressure and SoD as well as the shot particle shape, size and shot material(density). The result quality also depends on shot delivery system as there are different types in the state-of-the-art. These systems are summarized below [12] [13]:

- Suction: Air is accelerated with pressure and given a high velocity. This high velocity creates a vacuum inside the gun and thus the shot particles start moving toward the accelerated air stream through the hose that is connected to the gun. High velocity air catches the shot particles and creates the jet. High velocity air accelerates the shot particles through nozzle and after nozzle exit.
- Gravity Suction: This system utilizes gravity to deliver the shot particles into the stream. As gravity is utilized, a requirement of gun direction is crucial as it should point out downwards.

- **Direct Pressure:** Shot media is contained in a pressure vessel, once the sand media is completely filled and valve is closed, the vessel is pressurized with air that is coming out of one of two hoses going out from Air Supply. The other is carrying the air to combine with pressurized shot media. After the shot media and air combine they move through the hose and while flowing through the nozzle, expansion of compressed air occurs which mainly accelerates the shot particles. The requirement of relocating the shot media after each operation by filling the vessel again with shot media is the main drawback of this system.

- **Dual Pressure Pots:** The main drawback of Direct Pressure System is resolved by placing a secondary vessel which fills the main operating vessel with shot media through a control system after each operation. This system eases the utilization and creates a more continuous procedure.

The four above-mentioned systems are shown in Figure 1.4

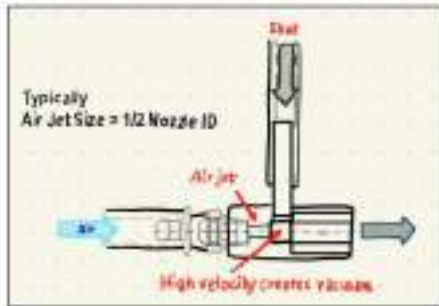
Shot Peening – Soft Blasting Applications

Shukla et al. [14] summarizes a general information on shot peening applications while comparing it with laser shock peening applications. It is stated that, average processing time for a single shot peening operation varies between 1 minutes to 15 minutes depending on the component with having a 11-14 € / hour of labour cost. Post-process step takes 15 minutes for cleaning and 30 minutes for a change over the machinery.

Shukla et al [14]. also presents a table that shows the main application sectors of shot-peening in different fields. Some of these applications can be seen in Figure 1.5

As the process motivation is different, application ranges of shot peening and soft-blasting also differ from each other. Some of the applications of soft-blasting are listed below [15]:

- Strips of paint and corrosion
- Cleans smaller tools
- Smooths and polishes devices
- Creates impressive art
- Cleans concrete surfaces
- Prepares surface for coating activity
- Restores authentic image of bricks and stones
- Enables mold remediation



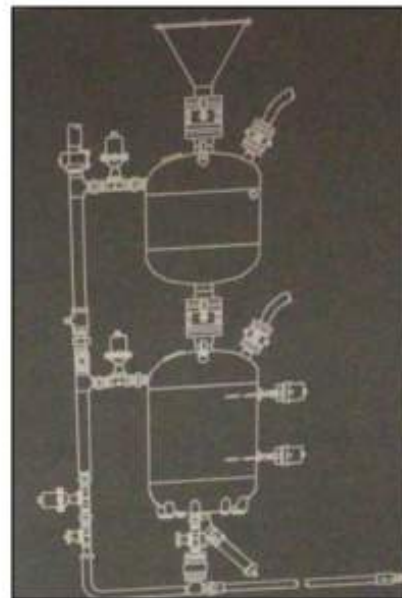
(a) Suction shot delivery system



(b) Gravity Suction system



(c) Direct pressure delivery system



(d) Dual pressure pots

Figure 1.4: Shot delivery systems [12] [13]

- Creates etched signs
- Removes oil stains from driveways

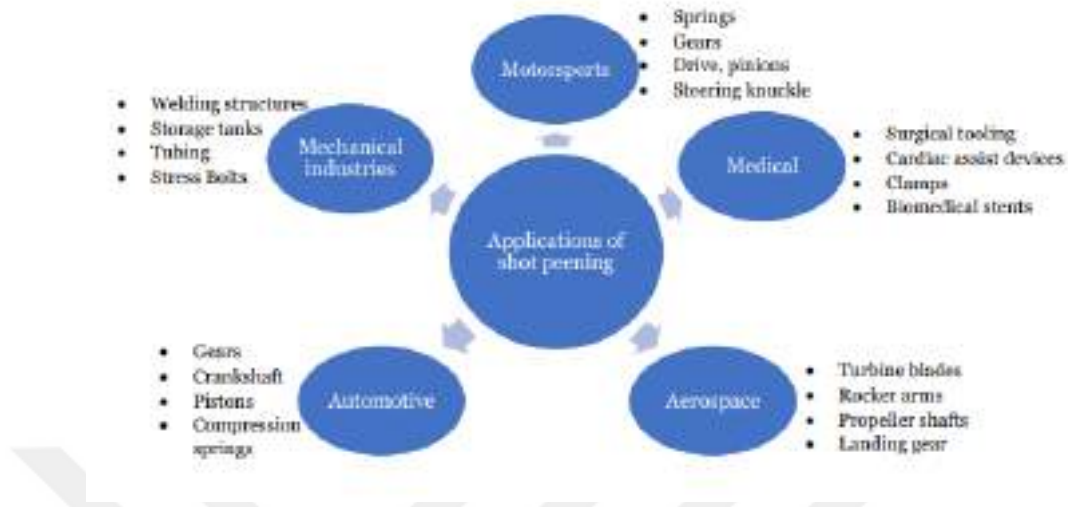


Figure 1.5: Various applications of shot peening[12] [14]

1.2 Literature Review on the Numerical Model of Peening/Blasting Processes

Shot peening numerical model is widely utilized in several scientific studies with different purposes. The main motivations include the examination of surface topography and residual stress state while varying several parameters of shot peening process like the time, coverage and shot velocity.

Several studies are done by Bagherifard et al. and these papers are examined as the main reference source at some steps of this thesis. For instance, a dimple regression idea is introduced in the paper dated in 2012 [16] in which surface roughness is examined both numerically and experimentally. The comparison results demonstrate that the maximum difference for Ra parameter is found as 11.7%.

Mesh convergence idea in the shot peening numerical model is introduced in a study of Bagherifard et al. dated in 2014 [17] where a critical mesh size that makes the results mesh-independent is evaluated.

Other studies that utilize shot peening numerical model and done by Bagherifard et al. focus on coverage assessment [18], prediction of surface layer after Severe Shot Peening (SSP) [1] and biodegradation acceleration and mechanical performance enhancement of pure iron after SSP [19].

Numerical model of shot peening is used in many other scientific studies as well. Below, brief explanations for these studies are given correspondingly.

Miao et al. [20] examines a FEM study on shot peening simulation. It is stated that unlike the shot peening numerical model studies in the literature, their study focuses on random impact locations for the impact sequence which is considered to let the model approach to experiment conditions.

The shots are impacted in two ways onto the surface of the substrate. These are normal direction (=90 degree) impacts and oblique direction (=60 degree) impacts. With random positioning sequence of the shots, the effect of impact angle is analyzed with their contribution to the results of arc height, coverage and roughness values. The idea is to relate these parameters to the number of shots for both impacting methodologies that mainly differ by the impact degree.

Results show that, number of shots for full coverage (=98%) are less for oblique impacts and normal impacts induce larger roughness value than normal impacts. It must also be stated that the examined surface roughness is indicated as PV roughness which is the difference between lowest valley and highest peak.

Study done by Bhuvaraghan et al. [21] utilizes Johnson-Cook material model to characterize substrate material and random impacting locations for shot peening. The examined parameter for surface roughness is Ra and it is shown that experimental approach gave the result of $0.776 \mu\text{m}$ and numerical approach gave the result of $0.649 \mu\text{m}$ which indicates a difference of 16.4%.

The numerical model introduced by Mylonas et al. [22] in 2011, is said to have some advantages from other publications like high number of shots in the simulation and shot dependency on the desired coverage. It is stated that 4 different shot types are utilized based on their sizes.

The results are also examined in the perspective surface roughness. The examined and indicated parameter for surface roughness is Rtm which is mentioned as average of highest and lowest points between dents. It is concluded that, Rtm increases with the increase in shot velocity. However, Rtm results do not show a good matching between numerical and experimental results and the percentage difference increases with the increase in the shot velocity. The paper states that even if the matching is not on a good level, the curve that Rtm values follow with regards to shot velocity is similar between numerical and experimental approaches.

The study done by Sanjurjo et al. [23] examines the effect of constitutive

material model used to characterize substrate in the simulation on the results of numerical model. The paper examines different material models like Johnson-Cook and Chaboche. It is stated that the proposed model by the paper demonstrates a good matching with the experimental results. The paper indicates the importance of strain rate effect in the material model.

Several other studies use Johnson-Cook material model including studies done by Jebahi et al. [24], Zhang, Proust and Retraint et al. [25], Hu, Tian and Wang et al. [26], Ren and Wang et al. [27].

The study done by Ghasemi et al. [28] states that the built numerical model examines the effect of coverage on surface state. Random impingement of shot particles is utilized. It is mentioned that, the results of numerical and experimental approaches have a good matching while a reduction of 25% in computational time and 80% in required RAM capacity is provided.

It is demonstrated that after 1000% coverage, the error percentage becomes 2.6% for Ra, 3.2% for Rq and 16% for Rt between numerical and experimental results.

Chen et al. [29] focuses on shot peening simulation on high manganese steel in order to see the effect of several process parameters like time, coverage rate and shot velocity on the compressive residual stress and surface roughness.

It is concluded that surface roughness (studied and indicated parameter is Ra) increases with process time, coverage rate and shot velocity.

Wu, Liu and Wei et al. [30] examines the residual stress and surface topography of carburized 18CrNiMo7-6 rollers after shot peening treatment. It must be noted that the surface roughness indicated parameters are designated S instead of R, that is the roughness is evaluated taking into account the surface in two directions but not single direction. The plots demonstrated in the paper with the purpose of comparing numerical and experimental findings, indicate a difference around 33% for Sa parameter. It is shown that, percentage difference tends to decrease while going up to 200% coverage level from 100% coverage level.

Khajehmirza et al. [31] also uses shot peening numerical model with the intention of estimating fatigue performance and surface state of shot peened laser powder bed fusion materials. The paper introduces a post-process algorithm to extract surface roughness parameters.

All of the above-mentioned studies are examined in detail during the

building process of the numerical model of soft-blasting in this thesis. The referenced sections of the model are correspondingly mentioned to cite the related papers.

1.3 Surface Morphology

Surface finish is one of the most important characteristics of the parts in the daily life since the quality of the surface texture identifies the interaction of the parts with its surroundings. Surface finishing operations define the final stage of manufacturing processes in order to obtain highest possible surface integrity [32].

The quality of surface morphology has the potential to influence several characteristic properties of the part like its friction properties or resistance to wear. As the future-concept of the topic studied in this thesis is wettability, it can also modify wettability [33].

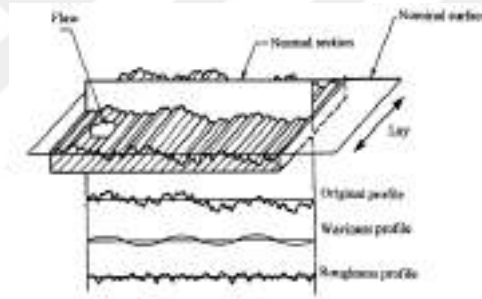


Figure 1.6: Roughness and waviness in a surface [34]

The primary profile of surface is mainly composed of two main contributions as indicated in Figure 1.6:

1. Roughness
2. Waviness

These two contributions simply sum up to form primary profile as it can be seen from Figure 1.6. One must know the distinction between roughness and waviness in order to examine them after specific heat treatment.

Roughness

Roughness is the lower wavelength elements inside the primary profile. The extraction of roughness requires high pass Gaussian filtering. With

this methodology, it is possible to delete longer wavelength data out of the primary profile data. The cut-off wavelength of the filtering operation is selected based on ISO-4288 and depends on the type of the machining process (periodic such as turning, milling, planing etc./non-periodic such as grinding, honing, lapping)[35] operated on the part.

Several parameters can be evaluated for characterizing the roughness. These values are examined more in detail in Step 2.6 in Chapter 2. To summarize, roughness is mainly characterized by parameters like the mean of absolute values of the entire data or their root mean square. Such other information like the highest peak-valley difference can also be utilized.

The evaluation length is also based on ISO 4288. Evaluation length is 5 times of the cut-off wavelength. Evaluation length is segmented into 5 for sampling purpose which makes sampling length be equal to cut-off wavelength. It is possible to extract the parameters as the mean of the calculations within the sampling lengths.

Waviness

Waviness is the higher wavelength contribution to primary profile. It is extracted in a similar way to roughness but as these are high-wavelength elements, waviness extraction requires low-pass Gaussian filter.

As the primary profile is mainly calculated by summing roughness and waviness, in order to evaluate surface roughness, one can also first utilize low-pass filter and extract waviness and then by subtracting this value from the primary profile, roughness can be evaluated.

These operations can also be done in 3D. As surface profile measurement terminology is built on 2D data, surface morphology parameters can be evaluated in both directions making the 3rd direction as the vertical profile displacement direction upon which roughness and waviness can be measured. However, for this purpose several pre-operations must be done. The most important operation is to tilt the surface to zero-surface of the plane formed by the measurement directions. More detail on this aspect will be explained in corresponding section of the thesis.

Chapter 2

Numerical Model Build-Up

2.1 FEA Reference Model for Shot Peening

A numerical model that simulates the shot peening operation with random impact sequence has been created and processed by several papers including [16][17][18][1][19] and [31]. Throughout the years, these and several other articles investigated different phenomena during shot peening with the numerical model routine like generation of surface roughness, mesh sensitivity, coverage assessment and different related cases.

The model used by Khajehmirza et al[31].is used as a reference model in this thesis. In that paper, shot peening is utilized to enhance surface quality of as-built Additive Manufacturing (AM) parts. A numerical model is used to estimate the resulting surface morphology and fatigue strength of parts after shot peening operation.

However, the concept of this thesis is not shot peening but soft blasting with different material sets and more irregular shot geometries. These differences require a different approach to build-up of numerical model where randomness should contribute on the impact sequence greatly. To fulfill this purpose, several updates have been done on the model.

To give the idea of all the updates done on the model, firstly the reference model should be explained in detail. In this section of the thesis, this reference model will be examined and in Step 2.5 of Chapter 2, the new model will be examined after covering the pre-processes done in Step 2.2,2.3and 2.4.

The reference model uses 3 main routines with the following identification:

1. MATLAB Randomness Generation Routine
2. ABAQUS FEA Model
3. Python Multiple-Impact Script Routine

All the steps and processes done in each routine will be explained step by step.

MATLAB Randomness Generation Routine

This MATLAB code is utilized to gather the required number of shot particles and their random locations over the substrate surface. It should be mentioned that all of the impacting particles are demonstrated as spherical parts in the study of Khajehmirza et al [31]. Using one single particle geometry without varying shape or size makes the sole use of single dimple throughout the complete model. A dimple is the deformed surface of substrate that has been formed because of compressive residual stresses created during the impact.

MATLAB code initializes with the evaluation of required shot number for given coverage level. Coverage is mainly the ratio of plastically deformed area to complete impact region area [18]. While assessing the coverage, Avrami equation is one of the equations that are mostly utilized which is as the following [30]:

$$Cov\% = 100 [1 - e^{-A_r}] \quad (2.1)$$

As it can be observed, there is a component A_r in Equation 2.10. This represents the area ratio upon which a coverage assessment will be done. This ratio is mainly the ratio of single dimple on the surface to the complete area of impact region. Equation 2.10 gives a number of particles for given coverage. However, this formulation can not go up to 100% coverage and thus a level of 98% coverage is considered to be valid [36].

Once the required shot number information is taken, MATLAB does all the remaining operations based on it. In fact, MATLAB randomly picks a point inside the impact region and identifies its boundaries as a circle and plots it. The coordinates of center point of the circle is recorded in a separate array.

After arranging the first particle MATLAB moves on with a while loop that works until reaching to the last particle. In every iteration of the while loop, a new sets of coordinates is obtained for new upcoming particle.

However, MATLAB must also avoid overlaps between particles. Thus, with including a series of codes, a validation step is taken into account in every iteration to check whether the current particle is at a distance away from the already selected circles.

To ensure that, a simple mathematical operation is done to see the distance between center of current circle and already selected circles. If all of these distance values are higher than a given threshold, then this point and thus the circle that will form around it will become valid and MATLAB will continue with the next iteration. The distance threshold is accepted as $1/3$ of dimple diameter that can be seen in Figure 2.1.

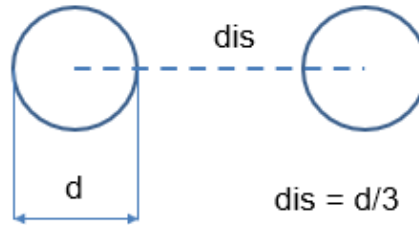


Figure 2.1: Representative of spherical parts distance threshold evaluation method

After all dimples and their locations are selected and listed, MATLAB plots the final image as can be seen in Figure 2.2.

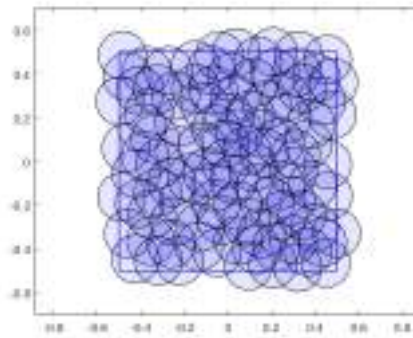


Figure 2.2: Cov 100% output for spherical shot media

Several comments should take place at this step about what to change in this MATLAB code in the concept of the thesis. As this reference model just works on spherical dimples, a modification should be done on this

perspective. The new model should therefore be able to detect and plot the boundaries of other chosen particle geometries.

Coverage assessment and overlap avoiding phenomena work on single dimension value. Coverage assessment takes the area of single dimple as an input whereas dimple diameter is the input for the process of avoiding overlap.

In the case of existence of many different geometrical shapes, all dimple shapes will differ from each other based on the shape, size and even the impact direction. The new MATLAB Randomness Generation code should take into account all the variety of dimple shapes and sizes. As the coverage assessment and overlap avoiding operations work on single dimension, MATLAB code should extract one single characteristic area and one single characteristic length dimensions to replace in the code.

The only randomness applied in this system is the random impact locations. However more randomness factors should be applied if the motivation is to approach to real-life operations like the random selection of shape and size of the particle from an already built group. Random rotation may also take place in the new model.

All the randomness factors that are used in the new model are examined in detail in Step 2.5 of Chapter 2.

ABAQUS FEA Model

For the Finite Element Analysis (FEA), ABAQUS Dynamic/Explicit is used. Here all the modules of the analysis will be briefly explained. 1-Part In Part Module, two parts are created as substrate and shot with specific dimensions. Substrate part is given face partitions and cell partitions in order to achieve desired meshing in the Mesh module where their visuals are shown in Figure 2.3.

2-Property

In the reference model, both substrate and shot is utilized as steel. The input parameters of both part sections include Density (tonne/mm^3), Young's Modulus (MPa) and Poisson Ratio except the plasticity parameters input for the substrate section.

As the shot impacts will plastically deform the substrate, plasticity of the substrate should also be included here. For this purpose, Johnson-Cook material model is used since this model can take high strain rate effect

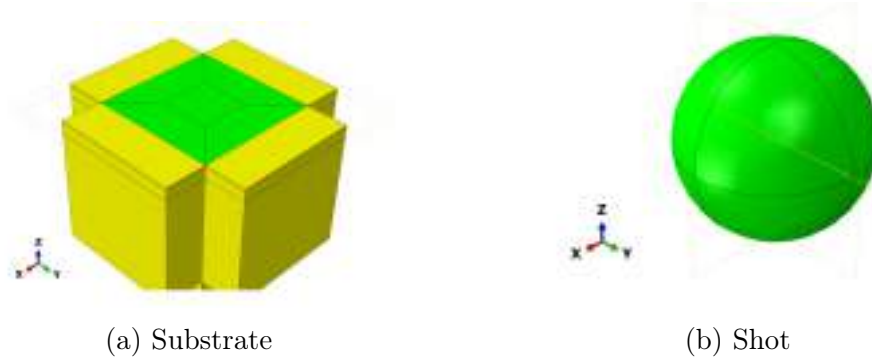


Figure 2.3: Reference model

into the model.

Johnson-Cook material model is mainly the Equation 2.2. [37],[38]

$$\sigma = [A + B\epsilon^n] \cdot \left[1 + C \ln \frac{\dot{\epsilon}}{\dot{\epsilon}_0} \right] \cdot \left[1 - \left(\frac{T - T_0}{T_m - T_0} \right)^m \right] \quad (2.2)$$

Johnson-Cook material model equation can be considered as 3 contributions. The first group is the main model, $[A + B\epsilon^n]$ where the data is extracted out of single stress-strain curve given for a specific strain rate and that specific strain rate becomes the reference strain rate of the entire model.

In main model contribution, parameters are listed as the following with their explanations.

- A: Initial yield of the material [MPa]
- B: Flow stress on strain hardening [MPa]
- n: Strain hardening exponent

The second contribution is the strain rate contribution. It is included in order to update the data based on stress-strain data of the material under different strain rates. In an operation like shot peening-soft blasting process family, high strain rates are expected to occur. Thus, the strain rates that are used while obtaining Johnson-Cook material model should also have high values so that the model can be valid at high strain rates. The important parameter in strain rate dependency contribution is as the following:

- c: Strain rate sensitivity

The last contribution is the temperature effect. Stress-strain data is also subject to change based on temperature variation. Thus, a contribution to

this issue must be included. These parameters are again obtained from stress-strain curves of same material under different working temperatures. These parameters are as the following:

m : Thermal softening parameter

T_{melt} : Melting temperature of the material [K]

$T_{glass/ref}$: Glass transition temperature of the material [K]

3-Assembly

Assembly is the module where shot is placed above the substrate. It must be located at the contact point and exactly at origin since MATLAB code assumes this point as the initial condition assigns the translation coordinates accordingly. A representative image from Assembly module of reference model can be seen in Figure 2.4.



Figure 2.4: Assembly module of Reference model

4-Step

Dynamic/Explicit is arranged with a total step time as $4E-06$ s. Field outputs are taken as CSTRESS, PEEQ, S, U, V at each time zone of $1E-07$ s, making 40 frames through one entire Job.

5-Interaction

A general contact is given for the analysis with a penalty of friction coefficient equal to 0.2 [19], [39]

6- Load

The only load applied is the impact velocity of the particle. It is defined as a predefined Field and assigned to the entire region of the particle on negative Y direction, towards the substrate surface.

7-Mesh

Meshing of the instances are completed in two steps. First step is to arrange the meshing as the combination of 3D stress and acoustic elements.

The side walls of the substrate instance are meshed with Acoustic elements. The regions that remain between those side walls and the complete region of the shot part is meshed using 3D stress elements. C3D8R elements are utilized here, these elements are 8-node linear brick, reduced integration with hourglass control.

Utilization of Acoustic elements is what gives this model its name as “Acoustic Model”. The reason for using Acoustic elements is taking the matter to the next step. The real intention for using the side walls is to assign Half-Infinite meshes to them as this type of meshes do not reflect stress waves back into the system. [Half-Infinite mesh 2 refs] In the next step of meshing, all FEA model is exported as an input model file. By replacing the Acoustic elements (AC3D8) with Half-Infinite Elements (CIN3D8) and inputting this new model file, the complete system is ready for Job submitting.

After all these steps are done, CAE file is saved and exited. This created CAE file will later work in collaboration with Python script.

The updates on ABAQUS FEA Model for the concept of the thesis should be clearly identified to be in complete collaboration with other routines. New ABAQUS model will have more than one type of shot particle instances. All the datas that are subject to change based on particle shape and size should be input in Python routine instead of ABAQUS routine. For instance, impact velocity shall change based on the random particle selection. So, it must be arranged in Python routine just like total Step time information which is also subject to change based on particle shape, size and velocity. New ABAQUS model and new Python script should take all of these updates into account.

Python Multiple-Impact Script Routine

The data obtained from MATLAB that will be processed in Python includes the location for all impact centers. Python code should work in such a way that it applies the shots consecutively at those points. The script starts with requesting 3 parameters from the user. These are:

1. Initial shot number
2. Maximum shot number
3. Number of CPU's to use during simulation

By being able to have the initial shot number as an input, user is able to start the simulation from a point where it stopped previously. This gives a

chance to compensate for any possible error that might occur.

Next process is to read the data from MATLAB. Once this data is taken as an input, it is first split as it contains two different information.

- Translation on X axis
- Translation on Z axis

AS it can be understood, substrate surface remains on a XZ plane on ABAQUS and the vertical impact direction is Y axis. Thus, random location translations should be done on X and Z axis.

That is how the script works for all of the particles. It mainly translates the part in 3D space, as with the information provided. It also gives a translation on Y axis. The main motivation of this translation is to avoid any initial contact between shot and substrate during the simulation. In the utilized CAE model, shot is located at origin and just above the substrate. So during the translation phase, shot particle is also moved upwards. Because as the impacting sequence processes some regions of the substrate surface will have upwards displacement. Thus, the shot particles start their movement from an elevated distance.

Once the script arranges the position of the shot, then it uploads the deformed substrate instance from the previous job file as the motivation is to see all consecutive impacts on the substrate. This is very crucial from the entire model since without this step, the complete model would be a series of single impact simulations instead of a multiple-impact simulation.

Then the code submits the job and waits for its completion so that the next shot particle can be initialized.

Python script terminates once it processes the last shot particle.

The differences that the new model should include based on the reference Python script is that, it should be able to process higher amount of data that will be obtained from MATLAB as there will be new randomness factors. In fact, the new script should arrange all the factors accordingly to ABAQUS interface.

It is already mentioned that, there will be different sets of shot particles based on their shape and size, so Python script should do all the necessary operations for all of these groups. As the complete model specifications on ABAQUS can be arranged over Python, all of the necessary and novel steps based on the reference script will be introduced and utilized. One other important contribution to the reference script should take into account

the space accumulation of Job files on the computer as the expectation is to have high space-demanding simulation files. The new script should also delete unnecessary Job files at some time after that simulation have terminated.

2.2 Step 1: Substrate Selection and Shot Characterization

2.2.1 Substrate Material Selection

Shot peening is a technique to alter surface properties with several possible motivations including enhancement of fatigue resistance and modification in surface morphology. It mainly includes substrate material and shot media. Shot media are accelerated towards the substrate to provide required interaction. Thus, the selection of the substrate material as well as the peening media is considered to be in important stage.

Soft-blasting and shot peening share the same terminology as they are from the same process family. In both processes, an accelerated shot media is impacted on a substrate to induce plastic deformation. To understand the difference between them, one must firstly understand the motivation and objective of each process.

Shot peening is mainly used for enhancement in fatigue resistance in the industry. However, there are many scientific articles and applications for other purposes such as surface finish modification. There have been scientific studies stating that surface finish directly relates to wettability of a material. [40] Out of these facts, it can be said that simulating shot peening can demonstrate results regarding wettability.

When the motivation is to enhance fatigue strength, general application is aimed for metallic alloys including steel components with steel or ceramic shot media. Yet for wettability purposes, polymers are one of the base materials to start with in this novel scientific era. Still, one must clearly identify its motivations to have a possible material list. In the case of wettability, question arises around where shall be a demand for reduced wettability. Water is truly the source of life but it can damage many mechanisms with several effects. It can damage electronical hardwares, it can create corrosion. It can even erase the color from a surface. So, wettability can be a demand almost in any sector. In daily life, polymer material family is the one that has possibly the widest range of usage. Considering all these

facts together, polymer material family is a perfect starting point for doing scientific researches on soft blasting with its effect on wettability. This idea is more highlighted when the immediate availability and low price of polymer materials is considered. After clarifying main material family for substrate media, next step is to clarify the next constraints to limit the wide range of polymers. At this point, the algorithm that is used in this thesis is that N. Raghupati proposed in his Master's thesis [12]. Here were given some limits for Young's modulus, yield strength and tensile strength with also specifying a ductile material. However, in current study, it is aimed to make material selection with not only considering material properties but also the application. Considering this, it is reasonable to think of a wider range of material list. However, the material property thresholds used by N. Raghupati were also made on a reasonable level considering the process limits of soft blasting. These thresholds and their explanations from that study are summarized below [12]

$0.3 \text{ GPa} < \text{Young's Modulus} < 3.5 \text{ GPa}$

$18 \text{ MPa} < \text{Yield Strength} < 70 \text{ MPa}$

$20 \text{ MPa} < \text{Tensile Strength} < 70 \text{ MPa}$

- Low yield strength to have permanent plastic deformation
- High ultimate tensile strength not to break the part
- High Young's Modulus to maintain original shape
- Being a ductile material

For material selection, Granta EduPack 2021 R2 software is used. Within this software, limits are input and results evaluated. It is observed that even if there are many materials in the list, some common materials that are widely used in daily life are out of the list. Therefore, it is decided to look for other materials as well. In this way, polyether ether ketone (PEEK) material is included into our list. For all the materials that have been found, the application information are gathered from Granta EduPack 2021 R2 software.

Full name of the materials listed in Table 2.1 can be found in Appendix A.1 with also their main applications

After figuring out the possible set of material list, next step was to look for market solutions. During this evaluation that led to find 18 materials in total, GRANTA EduPack 2021 R2 is used in widest material range, Level 3. This causes some materials in the list to be specific to their usage and creates a complex accessibility process. Initializing from the list in Table 2.1 all materials are searched on online shops in sheet/plate form.

Table 2.1: Possible polymeric materials for substrate material [Granta EduPack 2021 R2]

Name	Young Modulus[GPa]	Yield Strength[MPa]	Tensile Strength[MPa]
AES	2.16-2.3	43-49	47-53.9
ASA	1.51-2.34	35.9-38.9	27.6-51.7
PCTA	1.65-1.96	40.7-62.1	50.9-77.6
PCTG	1.74-1.83	42.7-47.1	49-55
PHA	3.5-4	35-40	35-40
PLA	3.3-3.6	50-55	55-72
SMA	2.34-3.24	35.9-55.8	53.2-58.6
TPU	1.31-2.07	36-42	31-62
ABS	2-2.29	29.6-44.1	30-50
PC	2.21-2.4	59-65	57.2-69
PE	1-1.14	18-20	20-31.7
PMMA	2.24-3.24	54-72	54-72
PP	1.6-1.78	35.4-38	36.2-49
PTFE	0.4-0.552	19.7-21.7	20.7-34.5
PVC	2.48-3.3	41.4-52.7	41.4-52.7
PVDF	2-2.5	23-50	24.1-50
PEEK	3.76-3.95	90-110	97-117
POM	2.6-3.2	57.2-71.7	71.5-89.6

The reason behind looking for the materials in sheet/plate form is to ease the process of soft-blasting. Once a material is obtained as sheet/plate form, the only possible pre-processing is to cut the samples into desired sizes and trim the flashes.

After examining online shops for material purchase in Italy, Table 2.1 is reduced to a material list with higher accessibility.

As explained in introduction Chapter, most FEA models that were previously built for shot peening, used Johnson-Cook material model [37],[38] for characterizing plasticity of substrate material. Although Johnson-Cook model is not the only solution for the characterization of plasticity, considering the high strain rates that occurs during soft-blasting, it is considered essential to continue with this material model in this study. It should be added that the Johnson-Cook model is among the few strain rate-dependent material models available in ABAQUS.

Initializing from Table 2.2, a research literature is done for evaluating Johnson-Cook material model parameters for the so-far selected polymers. This section happened to be one of the biggest challenging parts in all study

Table 2.2: Materials that can be found in sheet/plate form

Name	Young Modulus[GPa]	Yield Strength[MPa]	Tensile Strength[MPa]
ABS	2-2.29	29.6-44.1	30-50
PC	2.21-2.4	59-65	57.2-69
PE	1-1.14	18-20	20-31.7
PMMA	2.24-3.24	54-72	54-72
PP	1.6-1.78	35.4-38	36.2-49
PTFE	0.4-0.552	19.7-21.7	20.7-34.5
PVC	2.48-3.3	41.4-52.7	41.4-52.7
PVDF	2-2.5	23-50	24.1-50
PEEK	3.76-3.95	90-110	97-117
POM	2.6-3.2	57.2-71.7	71.5-89.6

since in many of the observations, it is clearly seen that Johnson-Cook material models are mainly meant to characterize metals. Very few studies demonstrated the model for polymers.

After examining high number of scientific researches, Johnson-Cook material model parameters were found for ABS [41], PC [42], PTFE [43], PMMA [44] and PEEK [45]. As Johnson-Cook material model is mainly evaluated with tabular data of stress-strain curves of a material under varying strain rates and temperatures, a fitting is done for material PP [46] for finding its Johnson-Cook material parameters.

Table 2.3: Johnson-Cook parameters of substrate materials

Material	A[MPa]	B[MPa]	n	m	C	$\dot{\epsilon}_0$	Reference
ABS	39	48	1.5	0.879	0.053	0.0008	[41]
PC	80	75	2	0.548	0.052	0.005	[42]
PP	19.5	20.05	0.6125	4.740	0.0323	0.001	[46]
PTFE	11	44	1	1	0.12	0.0033	[43]
PEEK	132	10	1.2	0.7	0.034	0.001	[45]
PMMA	357	90	4	0.74	0.077	1	[44]

Remaining with 6 possible materials in total, another decisive action took place. It is decided to take only one part out of this table for validating the results with experimental data considering the high amount of computational time during simulation. The other 5 materials are considered as the set of substrate materials in the future studies once the model is validated with already selected material. Selecting the specific

Table 2.4: Mechanical Properties of substrate materials

Material	$\rho[\text{tonne}/\text{mm}^3]$	E[MPa]	ν
ABS	1.02E-09	2200	0.35
PC	1.20E-09	2590	0.39
PP	9.03E-10	1475	0.403
PTFE	2.15E-09	420	0.45
PEEK	1.30E-09	3800	0.4
PMMA	1.19E-09	2855	0.36

material for the thesis concept was mainly done based on availability. Since PC was the material with highest possible volume in the lab, it was chosen as the substrate material.

2.2.2 Shot Particle Characterization

Building a numerical model of shots impacting on a surface requires particle geometry characterization if the motivation is to approach real-life results. Since surface morphology is the primary outcome of the study, it is of upmost importance to get the closest dimple shapes once impact has occurred. These dimple shapes and their vertical penetration information is greatly influenced by the shape and the size of the impacting particle. Several scientific researches have focused on particle characterization. Melentiev et al. [[47]] used SEM imaging of Aluminum oxide particles and captured 6 shape parameters as equivalent circle diameter, circumscribed circle diameter, aspect ratio, elongation, convexity and circularity to describe particle shape characteristic distributions. It has been proven that there must be at least two shape parameters such as aspect ratio and square root of form factor to describe particle shape characteristic. Hentschel et al. [[48]] mentions that correlation between parameters clearly show if there is relation between shape parameters. A novel technique is used by Bowman et al. [[49]] which is taking benefits from Fourier descriptor. They introduce this technique to provide better acquisition of triangularity, elongation and squareness. Furthermore it is clear that sphericity, roundness and roughness has significant effect on shape descriptor. In the study of Berrezueta et al. [[50]] new parameters are also studied including fractal dimension, solidity,

Wadell's roundness, perimeter-area and sphericity. Nevertheless in many researches, particles are classified into 4 to 10 different shapes. However, Blott et al. [[51]] uses new ratios like I/L ratio (elongation ratio) and S/I ratio (flatness ratio) and it allows to classify particles in 25 different classes. In some cases, it is hard to scan the particles in 3D manner due to high cost, then 2D SEM imaging is used. In order to improve accuracy of the results, new sphericity class is developed which is used to differentiate spherical to flat and ellipsoidal to elongated particles.[[52]] In another study it is shown that, from a digital image, by defining only three shape characteristics as convexity, sphericity and aspect ratio, particle shapes can be evaluated.[[53]] In another conceptual study, the effect of roundness and sphericity on shape characteristics is studied by Power classification method.[[54]]

To account for geometry variation of the particles, an algorithm is built as in Figure 2.5 where series of processes are done consecutively starting with Scanning Electron Microscopy (SEM) analysis where particles are visualized with high magnification values. Alumina powder is one of the powders that

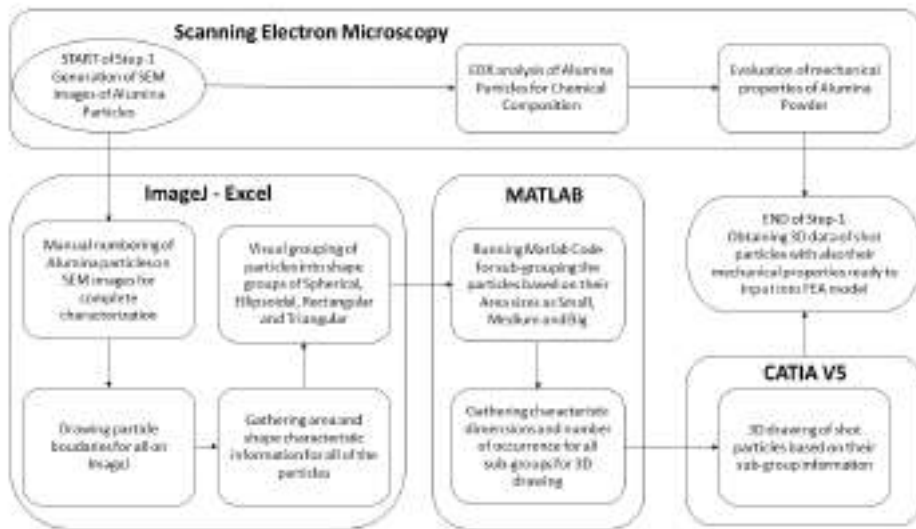


Figure 2.5: Algorithm of Numerical Model Step 2.2

is commonly utilized in soft-blasting applications. The ceramic of Al_2O_3

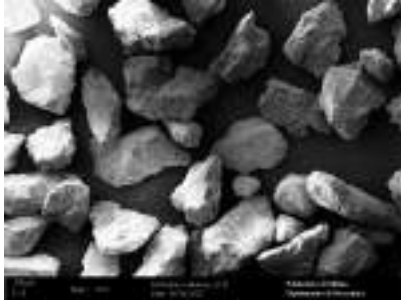
with its high strength and hardness combined with its physical stability is chosen here again for the shot material. A handful sample of the powder is taken from the soft-blasting machine for SEM analysis as well as EDS (Energy Dispersive X-Ray Spectroscopy) analysis. The purpose of EDS analysis was mainly to get the information of Alumina density inside the powder which can greatly influence mechanical properties.



Figure 2.6: Alumina Powder

A small amount of particles (as much as to cover finger-tip) is put on a flat plate in the size of a coin. To have better visualization, particles are coated with gold to ensure higher conductivity. However, another sample is also prepared without gold coating specifically for EDS analysis. The difference on visualization can be observed in Figure 2.7 where two SEM images are put to see gold-covering effect.

As Figure 2.7 shows, it is still possible to correctly see particle shape and observe its area. Considering this, SEM images without gold coating that are mainly intended for EDS analysis are also used in particle characterization step.



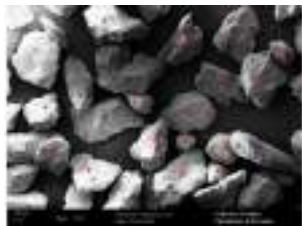
(a) Alumina SEM image with gold coating



(b) Alumina SEM image without gold coating

Figure 2.7: Representative SEM images with gold coating [left] and without gold coating [right]

After obtaining all of SEM images, a manual numbering is done for observing all the particles without any overlap between images. The images are taken from different regions of observation plate but since the observation area is particularly small, too many overlaps occur between images as expected. With doing manual numbering on all of them, overlap problem is overcome and total number of observed particles are evaluated as 210. ImageJ v1.52a software is utilized to get the dimension information of particles. This software makes its own numbering different from manual numbering previously done. A matching needs to be done to process the results in MATLAB. After numbering phase is complete, boundaries are drawn on each particle shape in ImageJ completely manually. Then, ImageJ is able to consider them as particles and give their dimensional information such as area, perimeter, circularity and roundness.



(a) Manuel Numbering



(b) ImageJ Numbering



(c) Binary Image

Figure 2.8: ImageJ processing; manual numbering [left], imageJ numbering [middle], binary image [right]

The best utilization of ImageJ in a context like the one in this study, is to make an automatic selection of boundaries based on light intensities of

SEM images. This is also tried in this study but as the intensities between regions with and without particle do not have very sharp and selective differences, this methodology did not work. For this reason, boundary selection is done by manual drawing.

The most important issue in particle characterization is obtaining 3D representative datas of particles out of SEM images which provide mainly 2D data. One has to make and list the assumptions going from 2D data to 3D data. First of all, a visual inspection is done on SEM images and 4 main particle shape categories (will be referred as “Groups” in this study) are decided as:

- Spherical
- Ellipsoidal
- Rectangular
- Triangular pyramid

For spherical and ellipsoidal particles, Obtaining area information is enough for 3D representation. Another set of assumptions are needed for 3D representation of rectangular and triangular particles where surface area observable on SEM images is not enough.

For rectangular particles, the base surface of the part is assumed to be square after visually observing occurrence of square shapes on SEM images as well as rectangular shapes. This group of particles will be represented as a rectangular prism which will have a rectangle surface and square surface. Taking the mean surface area of all the particles that fall upon this group out of ImageJ, the edges of rectangle surface will be listed and the smaller edge will form a square on the base surface. For triangular particles, assumptions required more information. For this purpose, ImageJ informations are imported into MATLAB and different set of possible correlations are observed between different parameters. When circularity is plotted against axis difference (difference between major axis and minor axis of the ellipse that is inscribed between the drawn boundaries of the particle in ImageJ), an exceptional behavior is observed. Whenever axis difference tends to increase, circularity tends to decrease and show a negative behavior.

Out of this concept, a cross correlation table is plotted for all the parameters and correlation between circularity-axis difference and roundness-axis difference are observed close to -1.

In other words, this study showed that when the particles in SEM data set start lowering their axis difference (aspect ratio can also be considered) they become rounder or the least round particles in the data set are expected to have higher aspect ratio. In the selected groups of 4 shape categories,

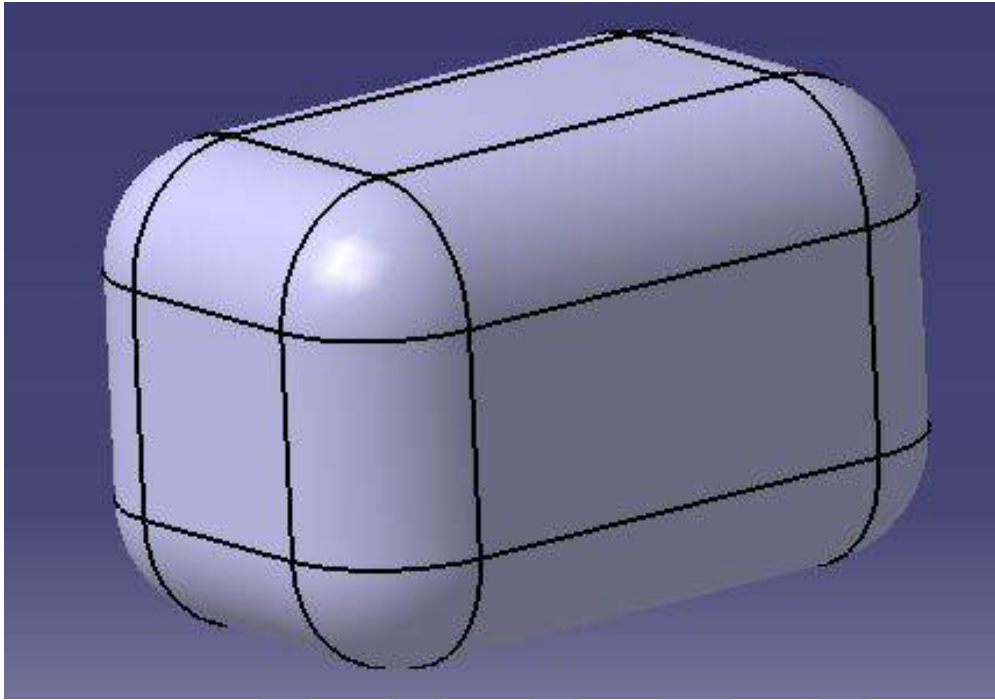


Figure 2.9: Rectangular Part drawn on Catia V5 R19

triangular particles are the ones to be expected with lowest roundness and circularity. Utilizing this information, led the way for another assumption. It is not expected to see equilateral triangles with high occurrence in SEM images yet they exist. So, 3D representative data for triangular particles are planned as a triangular pyramid which has isosceles triangles on 3 side surfaces and an equilateral triangle on base surface to cover for its less possibility of occurrence. 3D visual of triangular particle is shown in Figure 2.12

Grouping the particles based on selected geometrical shapes is an effective way to approach to real life model but yet not enough. Size average of each of particle groups can also be another varying prospect. That is a sub-categorization of the particles (will be referred as “sub-groups” in this study) is considered between each shape groups based on the area information obtained from ImageJ. A MATLAB code is utilized to take the $1/3$ and $2/3$ thresholds of area range between each group and sub-group them as:

- Small
- Medium
- Big

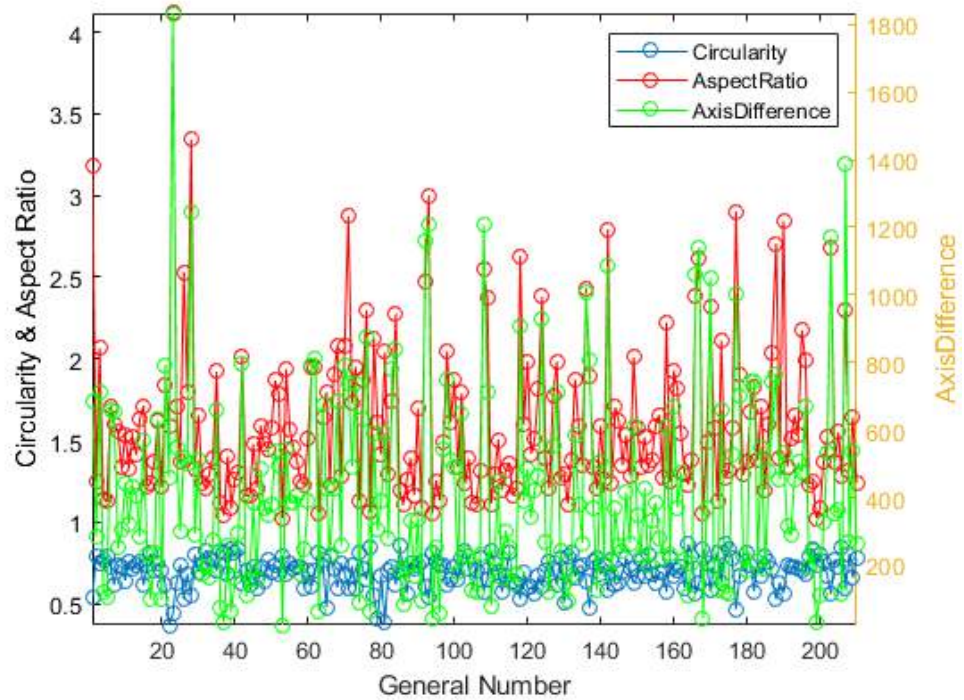


Figure 2.10: Circularity - Aspect Ratio - Axis Difference Plot through all 210 particle measurements

	1	2	3	4	5	6	7	8	9	10
	Area	Perimeter	MajorAxis	MinorAxis	Angle	Circularity	AspectRatio	Roundness	Solidity	Axis_Difference
1 Area	1	0.6034	0.6119	0.0506	0.0584	-0.0084	0.0768	-0.0616	0.1015	0.2267
2 Perimeter	0.9485	1	0.9206	0.7074	0.0713	-0.3752	0.3519	-0.3476	-0.1476	0.5661
3 MajorAxis	0.0810	0.0204	1	0.5868	0.0027	-0.0284	0.5452	-0.3140	-1.4826e-04	0.6150
4 MinorAxis	0.0504	0.0204	0.5868	1	-0.0076	0.2179	-0.4819	0.4140	0.1892	-0.0052
5 Angle	0.0544	0.0713	0.0817	-0.0076	1	-0.0740	0.0878	-0.3095	-0.0277	0.1135
6 Circularity	-0.0084	-0.3752	-0.0284	0.2179	-0.0740	1	-0.0400	0.0136	0.7873	-0.5990
7 AspectRatio	0.0768	0.3519	0.5452	-0.4819	0.0878	-0.0400	1	-0.0419	-0.1615	0.0910
8 Roundness	-0.0616	-0.3476	-0.3140	0.4140	-0.3095	0.0136	-0.0419	1	0.1948	-0.0447
9 Solidity	0.1015	-0.1476	-1.4826e-04	0.1892	-0.0277	0.7873	-0.1615	0.1948	1	-0.1130
10 Axis_Difference	0.2267	0.5661	0.6150	-0.0052	0.1135	-0.5990	0.0910	-0.0447	-0.1130	1

Figure 2.11: Cross-Correlation Table between ImageJ Parameters

Having done this sub-grouping leads to a 12 different particle sub-groups to 3D represent in total can be seen in Figure 2.13.

Same MATLAB code is further utilized to derive the required dimensional information for each sub-group. Set of required parameters can be seen in Figure 2.14

Obtaining these datas are crucial to be able to successfully 3D represent

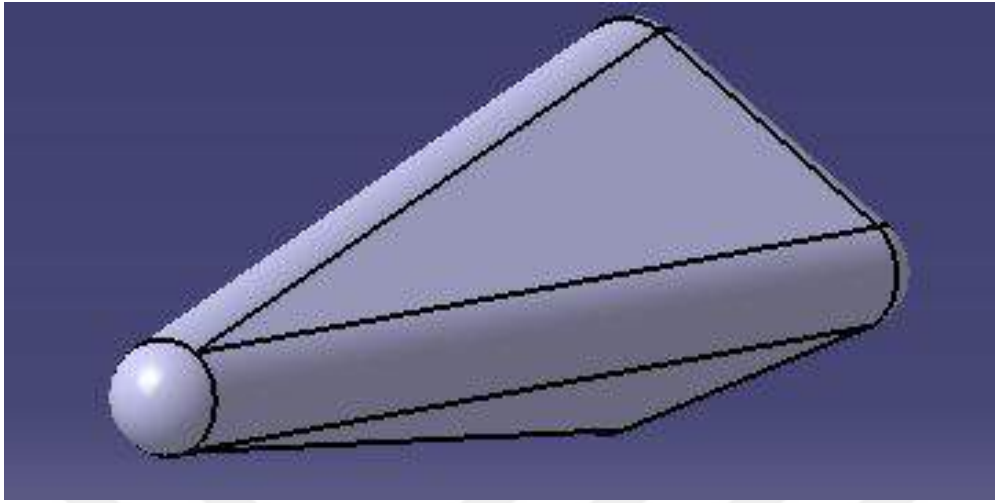


Figure 2.12: Triangular Part drawn using Catia V5 R19

particles. MATLAB code also counts the number of particles in each sub-group for assessing weight percentages while random assignment of particles will take place in Step 2.5, Chapter 2.5.1 of this study. Once MATLAB code completes its progress, every required information is ready to be input to any CAD software in order to 3D draw particles. In this study, Catia V5 R19 is utilized to draw shot particles.

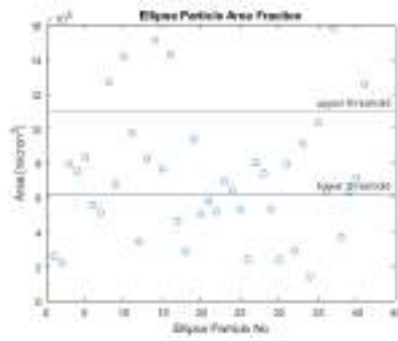
As Figure 2.15 shows there is also another contribution to final phase of this Step by series of EDS process blocks, this contribution mainly contributes to Step 2.5 where FEA model is built and shot material properties are required.

EDS analysis is done on set of SEM images to evaluate the percentage of alumina in the powder. The existence of other materials have the possibility to modify mechanical properties of shot media. EDS analysis can be seen in Figure 2.15 on complete set and on specific points. The material percentages on those analysis can be seen in Table 2.5

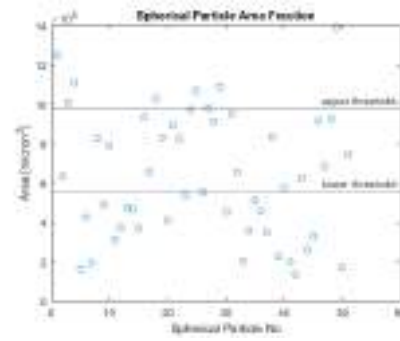
Table 2.5: EDS results of Alumina powder

Spectrum/Weight%	O	Mg	Al	Si	Ca	Ti	Fe	Total
Point A	44.30		55.70					100
Point B	47.30	4.41	10.18	3.60	0.90	26.03	7.77	100
Total Area	42.04		48.80	4.22	1.93	3.01		100

As results for Alumina percentage in complete visuals are around 90% -



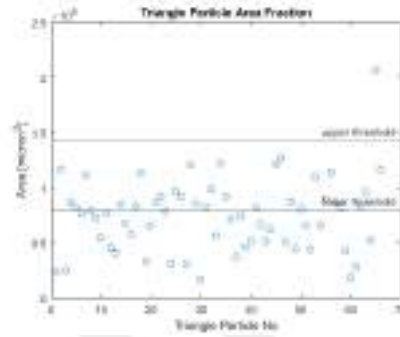
(a) Ellipsoidal Particle Area Distribution



(b) Spherical Particle Area Distribution



(c) Rectangular Particle Area Distribution



(d) Triangular Particle Area Distribution

Figure 2.13: Particle area distribution of each individual characteristic shape

91%, Alumina material reference is obtained from Granta EduPack 2021 R2 as material Alumina (90% with required mechanical properties to FEA model summarized in Table 2.6

Table 2.6: Mechanical properties of Alumina fraction 90%

	$\rho[kg/m^3]$	E[GPa]	ν
<i>GRANTA EduPack 2021 R2</i>	3.45E3-3.6E3	260-312	0.21-0.22
Selected Mean Values	3.525E3	286	0.215

Total number of particles in each group and sub-group are also presented below in Figure 2.16 and Figure 2.17 with histograms and pie-charts and all the characteristic dimensions with combining total particle number is given in Table 2.7.

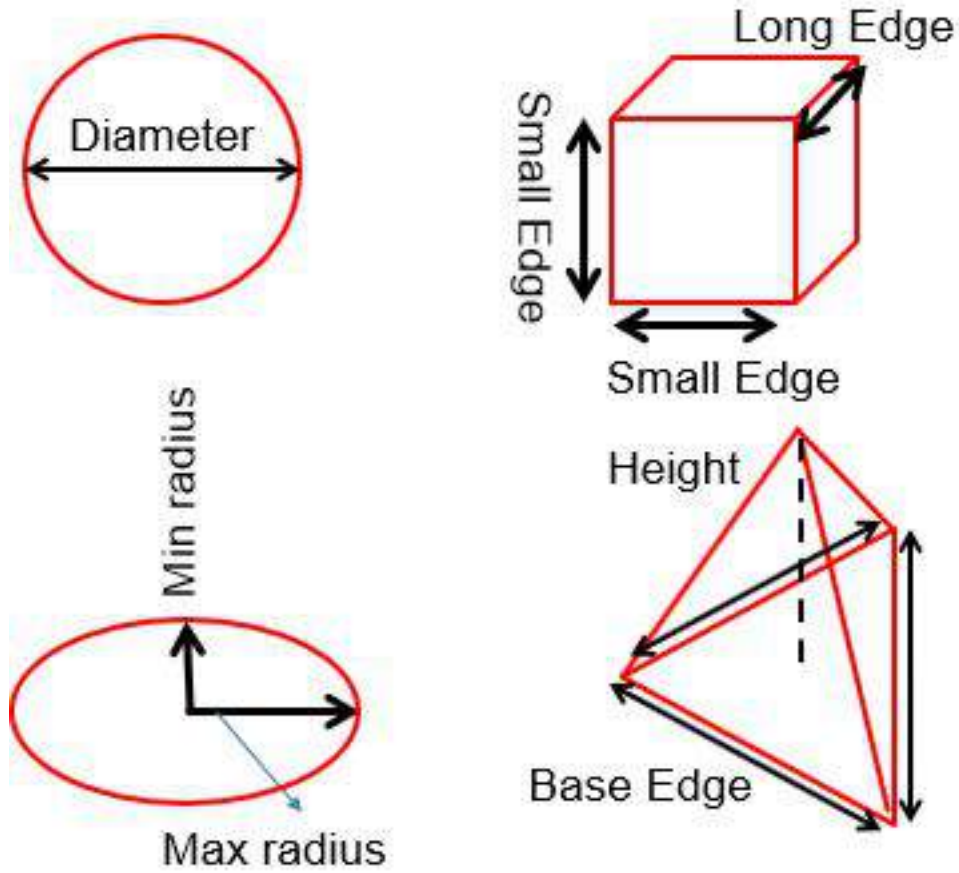


Figure 2.14: 3D characterizing information for particle groups

This ends the Step 2.2 of Numerical Model Build-Up after having obtained both mechanical properties and 3D information of shot particles.

2.3 Step 2: Impact Velocity Range Evaluation

Chapter 2.2.1 clarifies the required inputs that Soft-Blasting machine requires when operating on it. N.Raghupathi [12] used exactly same machine parameters in the set of experiments as Air Pressure (P), Stand-off Distance (SoD) and Impact Time (t).

Chapter 2.3 explains the FEA reference model for shot-peening upon which soft-blasting model is being constructed. It can be observed that, in the Loading module the only input is impact velocity of the particle.

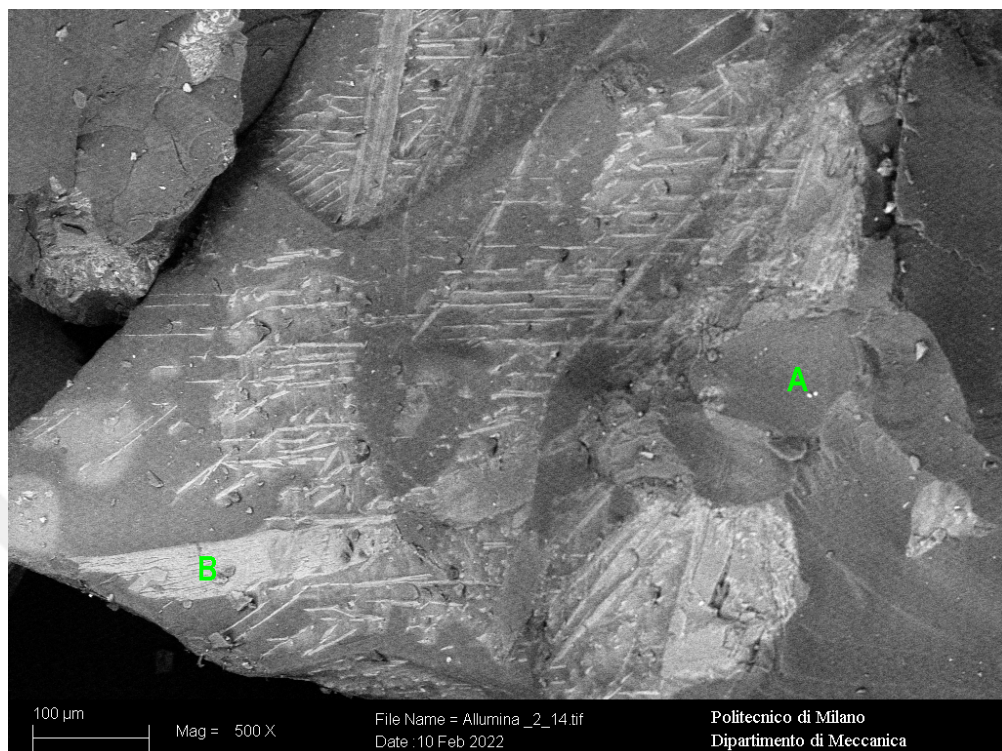
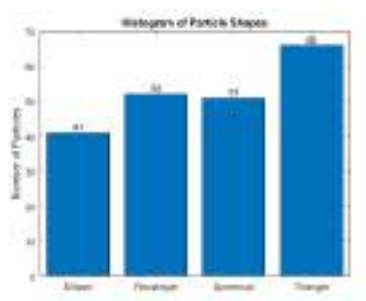
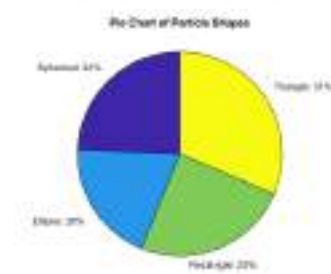


Figure 2.15: Representative visual of point A and B from Table 2.5



(a) Group histogram chart

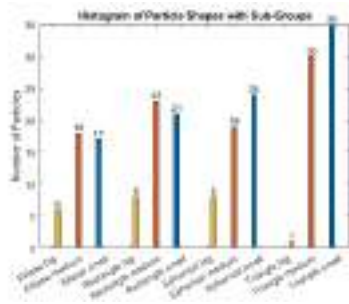


(b) Group pie chart

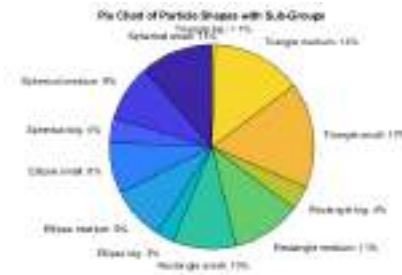
Figure 2.16: General shape group

Impact velocity values are quite large and the impact region is dusty. Thus, it is very hard to measure the impact velocity in real-life operation by examining particle movement during impact. This brings the ultimate requirement of relating the real-life machine parameters to impact velocity that will be input to FEA model.

If such a relation model can be succeeded, a consecutive data set between



(a) Sub-Group histogram chart



(b) Sub-Group pie chart

Figure 2.17: General shape sub-group

Table 2.7: Dimensional information for all particle sub-group

Particle Group	Size	Diameter[μm]		Total Number
Spherical	Small	669.05		24
	Medium	1008.6		19
	Big	1190.7		8
	Size	Min. Radius[μm]	Max. Radius[μm]	Total Number
Ellipsoidal	Small	264.44	468.41	17
	Medium	366.51	683.79	18
	Big	534.64	841.61	6
	Size	Small Edge[μm]	Long Edge[μm]	Total Number
Rectangular	Small	565.74	874.18	21
	Medium	675.37	1280.9	23
	Big	878.3	1443.7	8
	Size	Base Edge[μm]	Height[μm]	Total Number
Triangular	Small	777	1332.9	35
	Medium	1060.7	1839.4	30
	Big	1341.1	3077.9	1

Experimental Input	FEA Input
Air Pressure	Impact Velocity
Stand of Distance (SoD)	
Impact Time	

Table 2.8: Input parameters

machine parameters and numerical model can be listed. This real life – numerical model coupling step over impact velocity is thus very important.

A wide research literature is done on this matter and 3 relevant papers are

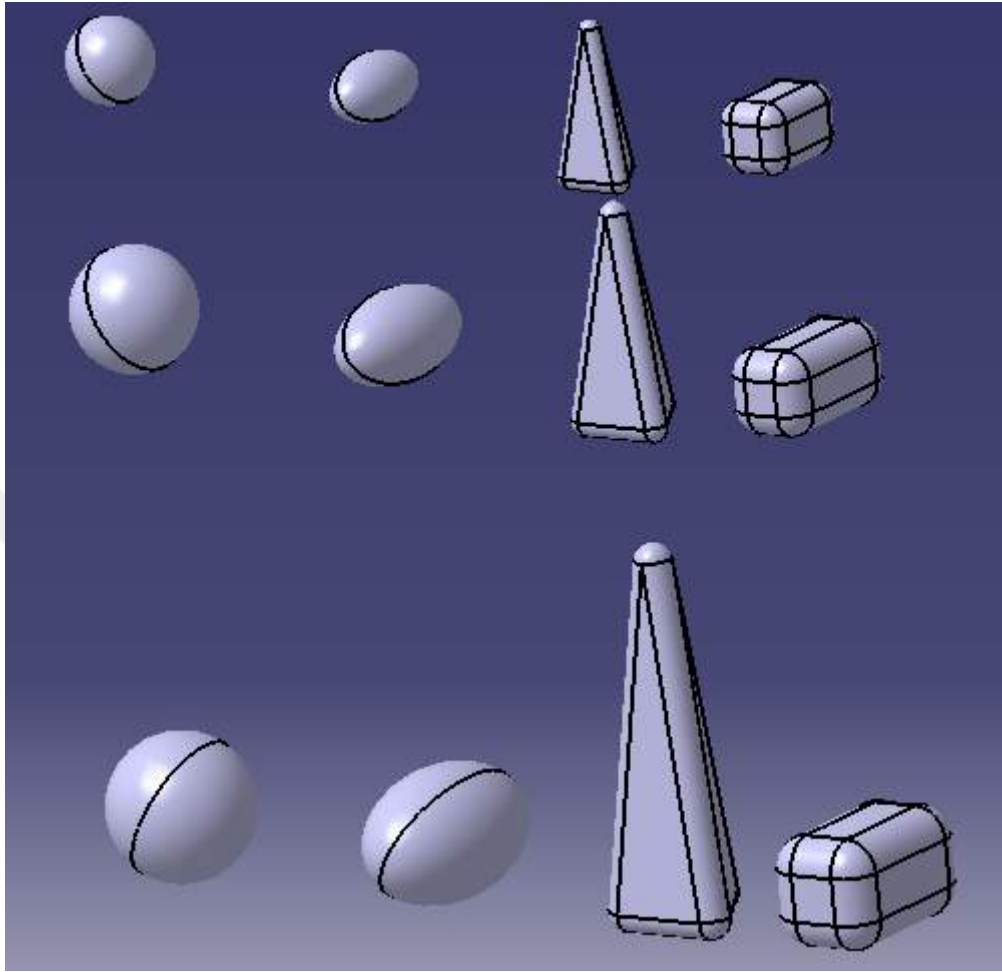


Figure 2.18: 3D visuals of all shots

found. These 3 papers construct on each other chronologically. Other than these, another paper dated in 2021 [55] also aims to develop a relation between Pressure and Impact Velocity. In this Step, they will all be explained briefly with their novel way compared to previous paper. Once their explanations are done, the algorithm built for Soft-Blasting numerical model will be explained in detail with all the formulations covered.

Kirk [56] explains the shot velocity creation with 3 main stages:

1. Air Stream
2. Shot particles introduction to air stream
3. Shot particles acceleration by air stream

As the main accelerator of the shot particles is air stream, it is needed to provide the velocity model of air stream. Air flowing through pipes is thus

modeled. However it is mentioned that, air velocity has a “sonic barrier” that could not be exceeded yet still affecting the shot particles acceleration by varying the air density at higher velocities. This paper includes the contribution of shot material density, shot size and nozzle dimensions.

Li et Al. [57] examines the abrasive particle velocity in Abrasive Jet Micromachining (AJM) and contributes to evaluation of shot impact velocity by segmenting the nozzle length and after-nozzle length into pieces and calculating the shot particle velocity in all of these consecutive segments. The reason of such an enhancement is that air acceleration does not remain constant after nozzle exit and loses its velocity as it moves forward.

Inside the nozzle, air has a speed limit (also referred to as Laval speed) which acts like a sonic barrier. Kirk defines that this speed limit is reached with pressure of 1.9 Bar. Shot is accelerated by the air velocity. Li et al [57]. calculates the final shot velocity at the end of each segment considering a constant shot acceleration in each segment. After nozzle exit, air velocity starts decreasing and thus decelerating shot velocity after a critical point. Once air velocity is calculated in a segment based on current distance to nozzle exit, shot velocity is calculated out of air velocity contribution. Shot velocity is calculated by taking the initial velocity as the final shot velocity at the previous segment.

Li et al. [57] plots the particle velocity as in Figure 2.19. It can be observed that particles behave in an expected way. They accelerate inside the nozzle (the region before point-0) and continues accelerating until some specific point where air velocity and shot particle velocity become equal. As air is accelerated by a given pressure it will continue accelerating for some more distance after nozzle exit but once it starts losing its velocity, two velocity values will equalize and the balance will continue through some distance (region point-3 between point-10). From that point on, air will continue losing its velocity and behave more like a decelerator on the shot particle. That way, shot particle will continue losing its velocity.

Figure 2.19 is plotted with having velocity values at different air pressures and nozzle dimensions. Li et al [57]. also make an experimental validation and observe that the velocity model results are in good range with experimental findings as can be observed in representative visual taken from the paper in Figure 2.20.

Liu et al. [58] further investigates this matter and makes a particular difference to the system provided by Li et al [57]. Liu et al [58]. mainly say that once air-shot stream leaves the nozzle and starts its path through

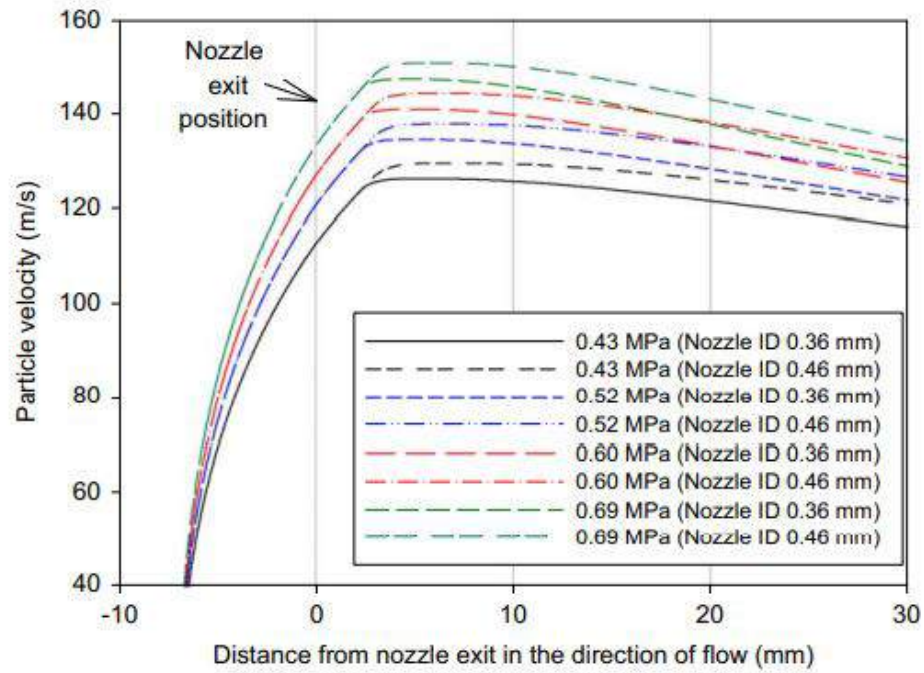


Figure 2.19: Velocity values at different pressure [57]

SoD, air density will also vary as the air pressure is the main contribution to define it. Using same segmentation logic provided by Li et al [57]. there is again a segmentation both inside the nozzle and after the nozzle in paper of Liu et al [58]. as well. For even better real-life approximation, it is mentioned the importance of varying air density variation into the system. Liu et al [58]. also provides an algorithm that defines the system very well. This algorithm can be seen in Figure 2.21.

These 3 papers construct a system in a chronological order to define a particle velocity that is accelerated by air stream under given pressure. Application of such a system is surely not limited to shot peening – soft-blasting process family as in many different machining processes, there may be air-accelerated-particles like in AJM.

Different than these 3 papers, another methodology is also examined by Wang et al [55]. To evaluate a relation between air pressure in real-life process and impact velocity in numerical model, a procedure is followed by making a series of experiments and simulations and measuring surface roughness parameters on the final surface morphology of both experimental and numerical processes.

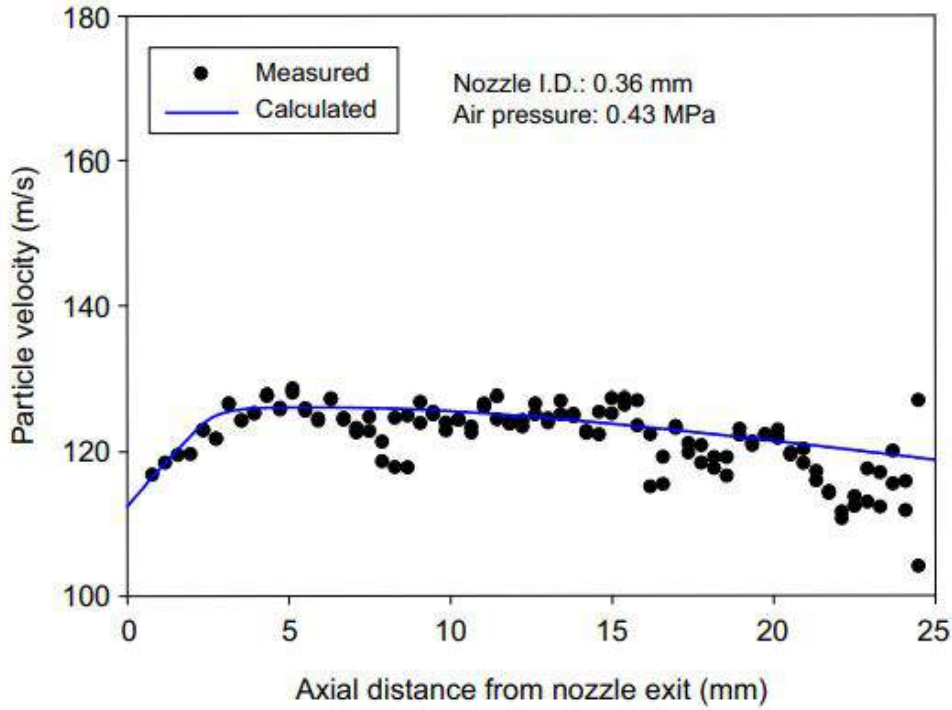


Figure 2.20: Velocity values validation with experiment [57]

The idea is to relate the pressure and velocity through final surface morphology. Surface roughness parameters are used as validation tool to obtain a mathematical relation between pressure and velocity.

This methodology provides a promising way to follow for particle velocity evaluation but as the concept of this thesis study is based on validating a new numerical model that is now taking into account the randomness of impacting particles, it is not reasonable to gather pressure-velocity formulation over a numerical model that is yet to be validated. A model creation in this perspective requires a direct velocity evaluation rather than finding a relation between pressure and velocity.

After examination of the articles, it is decided to follow the system chronologically defined by Kirk [56], Li et al.[57], and Liu et al. [58].

The system defined so far takes into account only spherical shot particles which does not match the requirements of this thesis. A new algorithm that is able to account for other groups of particles needed to be built.

The algorithm built for this thesis can be seen in Figure2.22.

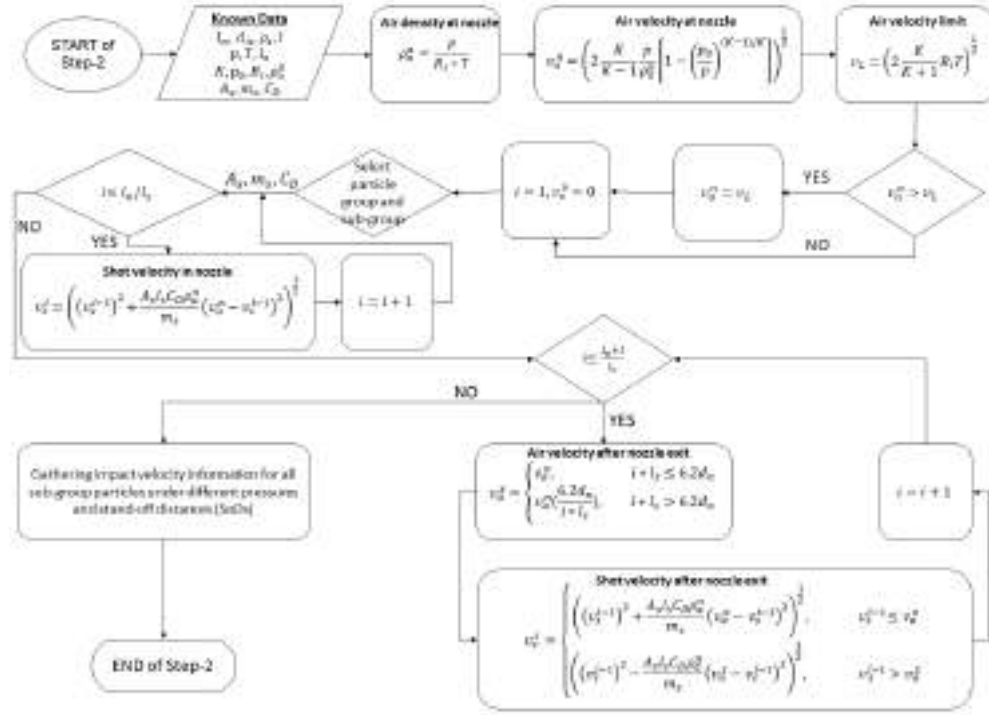


Figure 2.22: Algorithm of Numerical Model Step 2

$$p_a^n = \frac{p}{R_i * T} \quad (2.3)$$

Next process is to calculate air velocity in the nozzle with inputting adiabatic exponent of air and pressure of air both in nozzle and in ambient conditions.

$$v_a^n = \left(2 \frac{K}{K-1} \frac{p}{p_a^n} \left[1 - \frac{p_0^{(K-1)/K}}{p} \right] \right)^{(1/2)} \quad (2.4)$$

As explained before, air has a velocity limit in the nozzle. Air velocity that is calculated in the previous process must be compared with this limit velocity. If the air velocity is found out to be exceeding limit velocity, it should be taken as limit velocity as it technically can not exceed this limit value. Limit velocity can be calculated as in quation 2.5

$$v_L = \left(2 \frac{K}{K+1} R_i T \right)^{(1/2)} \quad (2.5)$$

Algorithm is followed by a decision where air velocity is accepted as limit velocity if it exceeds that limit value.

Then algorithm considers an initial velocity for the particle to be equal to zero and asks for an another decision about clarifying the group and sub-group of the particle. As there are 12 sub-groups of the particles in this study based on their shapes and sizes, velocity calculations must be done for each of the sub-groups.

The future processes will utilize the surface area, mass and drag coefficient of the particle. This decision step must provide these information to the next process block. In Table 2.9, formulations for surface area and mass can be found being evaluated by dimensional information of each particle that have been gathered in Step 2.2 of this study. Drag coefficient is also subject to change between each group of the particles. Table 2.9 also summarizes the drag coefficient information for each sub-group.

Once algorithm receives required information, it starts a loop until the end of the nozzle. In this loop, there are segments with length of 0.1 mm. As the total length of the nozzle is equal to 65 mm, there are a total of 650 segments inside the nozzle.

Algorithm evaluates the final shot velocity at the end of each segment. Initial velocity is taken as the final velocity of the previous segment. This way, shot acceleration is kept constant only inside the segment but not entirely in the nozzle. This is the novelty that Li et al [57]. have brought to this system. In all segments, shot velocity is increased by same air velocity value that is evaluated at previous steps. The main shot velocity evaluation equation can be seen in Equation 2.6

$$v_s^i = \left((v_s^{i-1})^2 + \frac{A_s l_s C_D \rho_a^n}{m_s} (v_a^n - v_s^{i-1})^2 \right)^{(1/2)} \quad (2.6)$$

Once segments reach to the last one and final shot velocity leaving the nozzle is calculated, this loop terminates and the second loop that is for evaluating the velocity after the nozzle begins.

This algorithm has two main differences from Liu et al [58] at this point. This study does not take into account the air density variation which Liu

Table 2.9: A_s, m_s and C_D information for complete particle set

Ellipsoidal						
	Small	Medium	Big	Small	Medium	Big
	Vertical			Horizontal		
A_s	$\pi * d_{min}^2/4$			$\pi * d_{min} * d_{maj}/4$		
m_s	$\pi * d_{min} * d_{maj}/4$			$(4/3) * \pi * d_{min}^2 * d_{maj} * \rho_{shot}/8$		
C_D	0.5			0.6		
Rectangular						
	Small	Medium	Big	Small	Medium	Big
	Vertical			Horizontal		
A_s	$small_{edge}^2$			$small_{edge} * long_{edge}$		
m_s	$small_{edge}^2 * long_{edge} * \rho_{shot}$			$small_{edge}^2 * long_{edge} * \rho_{shot}$		
C_D	1.05			1.05		
Triangular						
	Small	Medium	Big	Small	Medium	Big
	Vertical			Horizontal		
A_s	$base_{edge}^2 * \sqrt{3}/4$			$base_{edge} * height/2$		
m_s	$(base_{edge}^2 * \sqrt{3} * height/12) * \rho_{shot}$			$(base_{edge}^2 * \sqrt{3} * height/12) * \rho_{shot}$		
C_D	0.5			0.5		
Spherical						
	Small	Medium	Big	Small	Medium	Big
	Vertical			Horizontal		
A_s	$\pi * d_{shot}^2/4$					
m_s	$\pi * (d_{shot}^3/6) * \rho_{shot}$					
C_D	0.47					

et al [58] input to the system. The main reason behind this is that, varying air density requires an information of air density at the impact point. In other words, as air density inside the nozzle is known, Liu et al [58] inputs also the air density at the substrate surface and varies air density between this range and by specifying the SoD, gives the information of air density at that specific point. However, air density evaluation is not known at substrate in the concept of this thesis. Moreover, some basic trials showed that by assuming a reasonable air density on substrate surface and modifying the algorithm to account for air density variation, final velocities have changed with a very few degrees. Thus it is decided to not to take into account the air density variation after nozzle exit.

Another difference from Liu et al [58]. is that the algorithm in that paper Figure 2.21, calculates a final air velocity at impact point before initializing loop. This misleads the particle velocity development after nozzle exit.

Both Li et al [57]. and Liu et al [58]. demonstrated that air starts losing its velocity after a critical distance that is equal to 6.2 times of nozzle diameter. When air velocity after nozzle exit process block operates before loop, algorithm assumes a constant air velocity through complete SoD which is not the real-life case.

Air velocity shall vary between the value it has in the nozzle and the value it will have at the end of the SoD horizon. It should reflect the behavior of keeping constant until a specific point and then decreasing. This needs to input process block of air velocity after nozzle exit into loop unlike Liu et al [58].

As algorithm starts the second loop for shot velocity development after nozzle exit, first process is to get the information of air velocity at that specific segment. If the segment is at a distance lower than 6.2 times of nozzle diameter, air velocity is taken same as its value inside the nozzle. If this distance value exceeds 6.2 times of nozzle diameter, then air velocity is evaluated as in Equation 2.7.

$$v_n^a \left(\frac{6.2d_n}{i * l_s} \right), i * l_s > 6.2d_n \quad (2.7)$$

Once air velocity inside the segment is known, next process is to evaluate resulting shot velocity accelerated or decelerated by air velocity. This is decided upon the final shot velocity of the previous segment as its being greater or lower than the air velocity in the current segment.

Formulation in the process block of shot velocity in the nozzle also applies here, this time having the current air velocity as the accelerator or decelerator and still taking the final shot velocity of the previous segment as the initial velocity.

If the current air velocity is greater than or equal to final shot velocity of the previous segment, this will mean that air still has an acceleration effect on the particle and thus shot velocity will be evaluated with Equation 2.8.

$$\left((v_s^{i-1})^2 + \frac{A_s l_s C_D \rho_a^n}{m_s} (v_a^x - v_s^{i-1})^2 \right)^{(1/2)}, v_s^{i-1} \leq v_a^x \quad (2.8)$$

If the final shot velocity of the previous segment is greater than current air velocity, this will mean that air will have deceleration effect on shot particle and thus formulation will modify so to have a decreasing effect

and become Equation 2.9.

$$\left((v_s^{i-1})^2 - \frac{A_s l_s C_D \rho_a^n}{m_s} (v_a^x - v_s^{i-1})^2 \right)^{(1/2)}, v_s^{i-1} > v_a^x \quad (2.9)$$

Once loop reaches to the last segment and calculates the final shot velocity, it terminates. Having calculated this final shot velocity, motivation of Step 2.3 is fulfilled.

Some arrangements are done in complete algorithm of Step 2.3 as explained before to gather the velocity information under different air pressures and SoDs. For this purpose, total SoD is input as 500 mm in which algorithm calculates velocity development after nozzle exit. This is done mainly for being able to calculate shot velocities under different SoD until 500 mm over the same plot.

Air pressure is not input as one single pressure but rather a set of pressure values as they are between 2 Bar and 6 Bar. Having done this, written MATLAB code is able to give 5 plots all under different air pressures at the same plot.

As summarized in Table 2.8, real-life machinery has three main inputs as: Air pressure, SoD and impact time. Impact time technically has no effect on shot velocity but air pressure and SoD has their contribution on velocity development. MATLAB code written in this thesis to represent the algorithm built and modelled in Figure 2.23, gives the advantage of observing different shot impact velocities under different air pressure and SoD values on the same plot.

The only reason to require to run the code multiple times is the particle shape and size effect. Algorithm runs on a given particle shape and size. Code is enriched with the surface area, mass and drag coefficient information of all the particle sub-groups. By simply changing the shape and size name of the particle whose velocity is under evaluation, code is able to plot its velocity development.

A representative MATLAB code output can be seen in Figure 2.23 where green dashed line represents nozzle exit point and green dots are put to intersect velocity lines with nozzle exit. Red dots are the points where air velocity requires to be evaluated.

Gathering shot impact velocity for all sub-group particles under;

- Pressures: 2-3-4-5-6 Bar

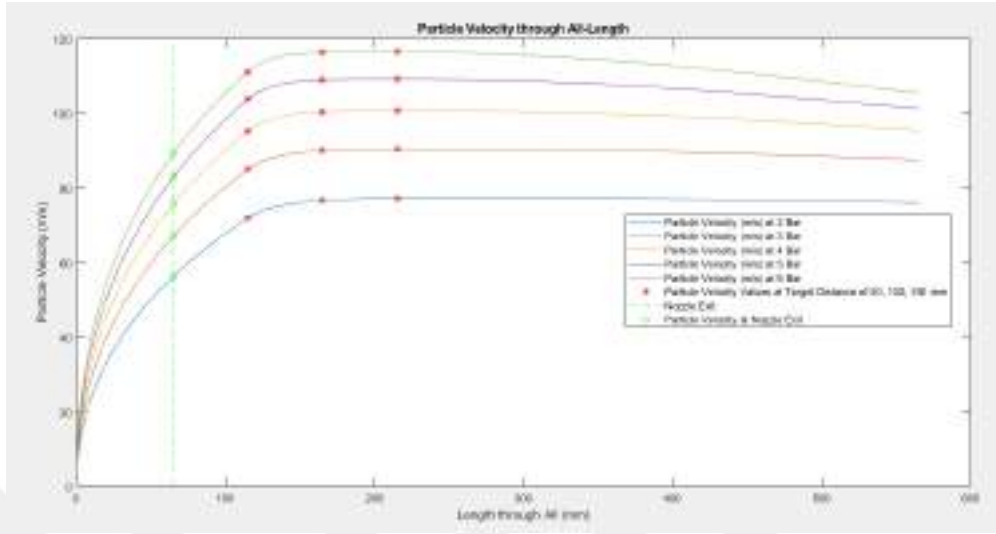


Figure 2.23: Particle velocity plots under different pressures

- SoD: 50-100-150 mm brings Step-2 to a close.

2.4 Step 3: Dimple Regression and Mesh Convergence

2.4.1 Dimple Regression

As explained in Chapter 2.3 where details of reference FEA model for shot peening have been examined, it is mentioned that evaluating the total number of impacting particles in a multi-impact environment is done by coverage assessment. The total number of particles for 100% coverage on impact zone is calculated in Step 2.5 of Numerical Model Build-Up. As it is mathematically impossible to reach to 100% coverage, a level of 98% coverage is considered [36].

The relation of coverage to this current Step 2.4 of model construction mainly includes dimple dimensions. The most basic question to answer is that; when shall model know it reaches 100% coverage and stop?

The answer methodology to this question relies on dimple creation phenomenon. More in precise, every sub-group of particles will have a characteristic dimple on the substrate surface with their own characteristic dimensions. In other words, all sub-group of particles will have a unique

deformed area after their impact on the surface.

The ultimate solution is to calculate coverage out of these dimple dimensions. The methodology about calculating coverage will be explained in detail in Step 2.5. This section mainly explains the dimple dimension extraction and their utilization.

This numerical model develops the already-developed models for shot peening process mainly by including randomness into the model. Already developed models were running the multiple impact simulations solely with spherical particles and with a fixed impact velocity. As the particle was a spherical part, any kind of random rotation was unnecessary as it would not alter the deformation on the substrate.

However, this new model has 3 main shapes other than spherical particle and also has sub-groups based on sizes of the particles. All of the randomness details will be explained in Step 2.5 but a particular case needs to be explained in this Step 2.4 which may be referred to as “Impact Singularity”.

Impact Singularity

A 3D particle visualized in Figure 2.24 has 6 degrees of freedom in space.

- Translation on X axis
- Translation on Y axis
- Translation on Z axis
- Rotation around X axis
- Rotation around Y axis
- Rotation around Z axis

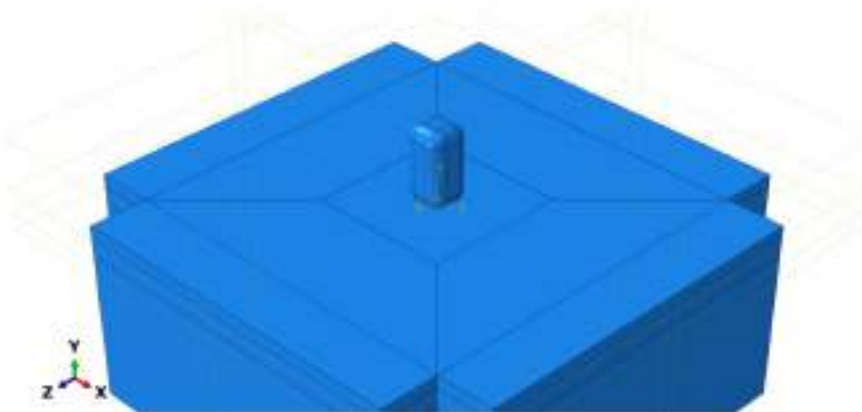


Figure 2.24: 3D rectangular part assembled on the substrate

As randomness is one of the most important contributions that this model makes to state of the art, all of these degrees of freedom must be examined.

Translation on X and Z axis are two parameters that are decided randomly on MATLAB routine applied in Step 2.5. These will locate the impacting particle on a random position above the substrate surface.

Translation on Y axis, is a fixed value that is manually decided in Python routine of Step 2.5, its main motivation is to hinder interference between impacting particle and substrate at the initial condition.

Rotation around Y axis is yet another random parameter decided in MATLAB routine of Step 2.5. It rotates the part around global-Y axis of the simulation while the particle is still at the origin. In other words, particle is rotated around Y axis before it is translated on X and Z axis leaving the main dimple shape unchanged but just rotated.

Rotations around X and Z axis are the main phenomenons that create impact singularities. As it can be seen from Figure 2.24, a rotation around Y axis, would not alter the dimple shape as it would still be a rectangle dimple on the substrate. However when the particle is rotated around X or Z axis, the dimple shape would not be a rectangle. In fact, depending on the degree of rotation around axis, there can be an infinite number of dimple shapes. This creates a problem for the complete model as it relies on coverage assessment in Step 2.5 which is characterized by dimple dimensions under all impacting sets. In other words, rotating the particle will create impact singularities and bring the model to an unsolvable statue. Thus, rotation around X and Z axis are ignored in this model.

However, as the main motivation is to approach to real-life process, an assumption is done to cover these rotations effect even if not best.

For every sub-group of particles except spherical particles, there assumed to be 2 impacting directions as called vertical and horizontal.

For ellipsoidal;

- Vertical impact means impact of sharp corner on the substrate
- Horizontal impact means impact of wider corner on the substrate

For rectangular;

- Vertical impact means impact of square surface on the substrate
- Horizontal impact means impact of rectangle surface on the substrate

For triangular;

- Vertical impact means impact of equilateral triangle surface on the substrate
- Horizontal impact means impact of isosceles triangle on the substrate

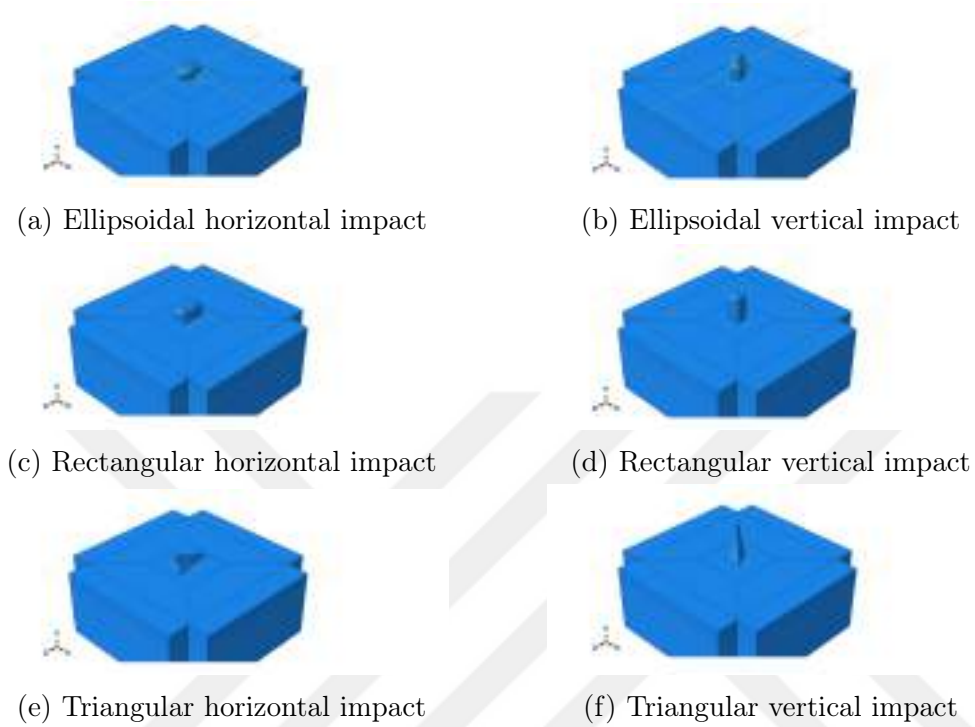


Figure 2.25: Ellipsoidal, Rectangular and Triangular particles impact direction visuals

These further impact direction classification required the creation of list of impact sets. With spherical particles, impact direction does not create any difference giving 3 impact sets in total specified only by the size (sub-group) of the particle. On the other hand, with ellipsoidal, rectangular and triangular particles there will be further classification of impacting direction giving 6 impact sets in total for each. Thus, there will be 21 impact sets in total in complete model as can be listed in Table 2.10

Dimple characterization shall be done for all 21 impact sets.

As in every step of Numerical Model Build-Up, there is an algorithm for this step of model explaining 3 main operations inside.

- Dimple Regression
- Step Time Evaluation
- Mesh Convergence

Algorithm can be examined in Figure 2.26

Table 2.10: Total impact number of each individual shape accordingly their direction

Ellipsoidal						
	Small	Medium	Big	Small	Medium	Big
Impact Direction	Vertical			Horizontal		
Impact Number	3			3		
Ell Total Impact	6					
Rectangular						
	Small	Medium	Big	Small	Medium	Big
Impact Direction	Vertical			Horizontal		
Impact Number	3			3		
Rect Total Impact	6					
Triangular						
	Small	Medium	Big	Small	Medium	Big
Impact Direction	Vertical			Horizontal		
Impact Number	3			3		
Tri Total Impact	6					
Spherical						
	Small	Medium	Big	Small	Medium	Big
Impact Direction	Vertical			Horizontal		
Impact Number	3					
Sp Total Impact	3					
All Total Impact	21					

The idea behind dimple regression is mainly referenced by Bagherifard et al.[16] where regression models are created in Minitab 15 to relate input parameters as shot dimensions and impacting velocity to output parameter dimple dimension.

Algorithm starts with known data as Impact Velocity Range evaluated in Step 2.3, Impact Velocity Range Evaluation; 3D data and material properties of shot particle sub-groups obtained from Step 2.2.2, Shot Particle Characterization; and substrate material properties obtained from Step 2.2.1, Substrate Material Selection.

Next process is to run a series of single impact simulations with all impact sets listed in Table 2.10. As explained previously, Bagherifard et al. [16] includes not only the shot dimension but also the velocity into regression

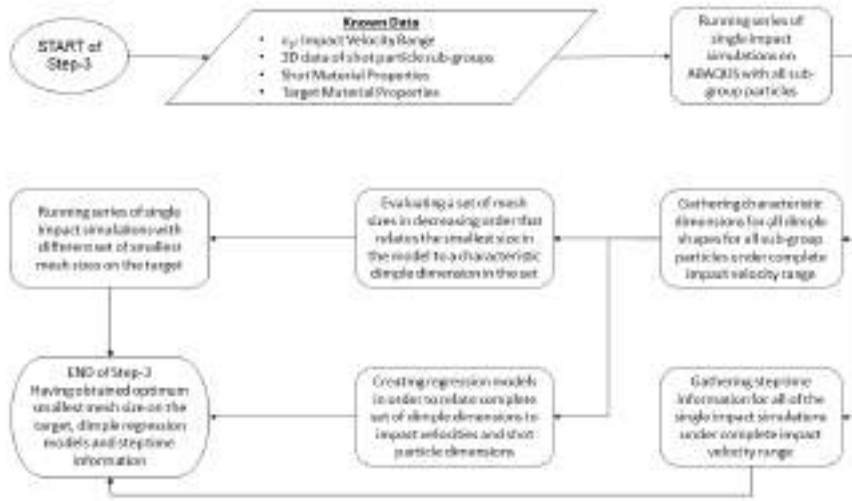


Figure 2.26: Algorithm of Numerical Model Step 3

models. Same methodology is also followed here. This required to run more than one simulations with same impact set under different impact velocities varying inside the velocity range obtained for that impact set in Step 2.3.

These velocities are chosen within the evaluated range. Taking a few degrees below the lowest velocity evaluated and a few degrees above the highest velocity evaluated and also taking a third velocity degree value as the mean of these two to increase the quality of regression is enough to create velocity range for series of single impact simulations.

Having 21 impact sets and 3 velocity values for each, 63 single impact simulations are done in order to gather dimple characterization.

Dimple characterization dimension selection is done with same perspective in Step 2.2.2, Shot Material Selection. For instance, as small edge and long edge dimensions are utilized to characterize the rectangular shot particle, rectangular dimple is also characterized by dimple small edge and dimple long edge. This creates yet another difference from reference models where the dimples are characterized only with one dimensional information, diameter of spherical particles, the shape that is solely utilized.

These multiple dimple dimension situation also alters the dimple regression models. Instead of having 2 inputs, one for shot dimension and one for velocity, in the dimple regression models of ellipsoidal, rectangular and

triangular particles there shall be 3 input parameters, 2 for shot dimensions and 1 for velocity.

Minitab is utilized here again for dimple regression models. Eventually there are 10 regression models in total for complete particle set as the following:

1. Dimple diameter regression for spherical particle
2. Dimple diameter regression for ellipsoidal particle vertical impact sets
3. Dimple minor diameter regression for ellipsoidal particle horizontal impact sets
4. Dimple major diameter regression for ellipsoidal particle horizontal impact sets
5. Dimple edge regression for rectangular particle vertical impact sets
6. Dimple small edge regression for rectangular particle horizontal impact sets
7. Dimple long edge regression for rectangular particle horizontal impact sets
8. Dimple base edge regression for triangular particle vertical impact sets
9. Dimple base edge regression for triangular particle horizontal impact sets
10. Dimple height regression for triangular particle horizontal impact sets

As can be observed from the list above, there are one dimple characterization regression for vertical impact sets since all vertical impacts create dimples that can be characterized by single set of dimensions.

Dimple regression models are given in Table 2.11. It can be observed that all regression models have R-sq values higher than 94% (except one rectangular) which ensures a good fitting of dimple dimensions through all impact sets.

Table 2.11: All dimple regression models with their R-sq values

Model	Impact Direction	Regression Model	Rsq[%]
Ellipsoidal	Vertical	$D_{min_D} = -0.224 + 0.001977V + 0.047S_{maj_D} + 0.700S_{min_D}$	96.37
	Horizontal	$D_{min_D} = -0.3032 + 1.285 S_{min_D} - 0.299 S_{maj_D} + 0.003233 V$	98.81
		$D_{maj_D} = -0.615 + 0.187 S_{min_D} + 0.681 S_{maj_D} + 0.004817 V$	98.3
Rectangular	Vertical	$D_{S_E} = -0.0231 + 0.001225 V + 0.8583S_{S_E}$	98.86
	Horizontal	$D_{S_E} = -0.0363 + 0.002937 V + 0.2490 S_{L_E} + 0.129S_{S_E}$	94.25
		$D_{L_E} = -0.901 + 0.00627 V + 0.457 S_{L_E} + 0.996 S_{S_E}$	87
Triangular	Vertical	$D_{B_E} = -0.177 + 0.6986 B_{E_1} + 0.001063 V$	98.37
	Horizontal	$D_H = -0.1053 + 0.8518 H + 0.2035 B_E + 0.000356 V$	99.99
		$D_{B_E} = -0.2976 - 0.0926 H + 0.9870 B_E + 0.001122 V$	99.47
Spherical	Vertical	$D_D = -0.1817 + 0.6336S_D + 0.002772 V$	98.1

2.4.2 Step Time Evaluation

A step time information is required to input to FEA model in Step module. That is the total simulation time of the model. The reference models have single particle shape, single particle size and single particle impact velocity which makes the step time unique for the reference model. However in the numerical model of this thesis, step time shall vary as all of its contributors vary.

Step time shall include the time that passes from the initial position of the shot until it reaches substrate as well. As specified before, a fixed value of Y position is given to hinder interference between shot and substrate. The required time that particle will travel this distance will vary based on the particle velocity.

As expected, step time shall also include total contact time of shot and substrate until the particle rebounds and completely loses the contact with the substrate. For this purpose, step time is input with high values in the series of single impact simulations that are mainly done for dimple characterization.

Once single impact simulations are complete, step time information is gathered for all of the simulations at the point where there is no more contact between shot and substrate.

It is observed at this point that, step time does not greatly change between different velocities of impact sets. Thus, it is decided to input the highest step time for each particle impact set.

When the Table 2.12 is examined, total number of frames needed to cover the time for the shot particle to rebound from the surface under different impact velocities can be seen. Frame means the time zone of $1\text{E-}07$ s. So, 10 frame means time zone of $1\text{E-}06$ s.

In this series of single impact simulations, shot particles are started at contact point with the substrate surface. So, resulting rebound frame only represents the total interaction time. However, particles will be initialized at an elevated distance above the substrate to avoid interference with the substrate. Considering this, an amount of additional frame must be input to cover these time zone. This additional frame is evaluated with applied velocity. Frame and additional frame sums to net frame that should be enough for the particle to rebound from the surface.

However in multiple impact environment, consecutive particles will not

impact on undeformed substrate surface like in the series of single impact simulations. This means that, particles rebounding frame may differ in later impacting sequences. Thus, an extra frame must be taken into account for this effect. This information is taken as 10 in this study.

Summing this extra frame, the input frame that should be included in Python routine in Step-4 is evaluated. These values are calculated for all impact sets under different velocities ranging from the lowest towards the highest while also considering their mean. These velocity values are all gathered in Step-2 of Numerical Model Build-Up. As the input frames do not greatly change between different velocities for most of the impact sets, input frame is taken as the highest value among the velocity range.

To summarize, a single step time information is evaluated in this way for all impact sets

These step time information can be examined in Table 2.12 , Table 2.13 , Table 2.14 , Table 2.15

Table 2.12: Step time information of Ellipsoidal shot

Ellipsoidal							
Shot	Velocity	Frame	Add. Frame	Net Frame	Extra Frame	Input Frame	Chosen Frame
Small-Vert	80	34	38	72	10	82	82
	100	33	30	63	10	73	
	120	32	25	57	10	67	
Medium-Vert	70	50	43	93	10	103	103
	90	48	34	82	10	92	
	105	48	29	77	10	87	
Big-Vert	60	66	50	116	10	126	126
	80	64	38	102	10	112	
	100	62	30	92	10	102	
Small-Hor	110	28	28	56	10	66	66
	130	26	24	50	10	60	
	150	26	20	46	10	56	
Medium-Hor	100	36	30	66	10	76	76
	120	36	25	61	10	71	
	140	36	22	58	10	68	
Big-Hor	80	54	38	92	10	102	102
	100	52	30	82	10	92	
	120	50	25	75	10	85	

2.4.3 Mesh Convergence

Mesh convergence is a procedure that needs to be examined in all FEA studies. As the parts that are under investigation are divided into high number of finite elements, size of these small elements greatly effects the results.

Table 2.13: Step time information of Rectangular shot

Rectangular							
Shot	Velocity	Frame	Add. Frame	Net Frame	Extra Frame	Input Frame	Chosen Frame
Small-Vert	100	30	30	60	10	70	70
	120	30	25	55	10	65	
	140	30	22	52	10	62	
Medium-Vert	80	40	38	78	10	88	88
	100	40	30	70	10	80	
	120	40	25	65	10	75	
Big-Vert	80	44	38	82	10	92	92
	100	44	30	74	10	84	
	120	44	25	69	10	79	
Small-Hor	110	26	28	54	10	64	64
	130	26	24	50	10	60	
	150	26	20	46	10	56	
Medium-Hor	100	32	30	62	10	72	72
	120	32	25	57	10	67	
	140	32	22	54	10	64	
Big-Hor	100	38	30	68	10	78	78
	115	40	27	67	10	77	
	130	40	24	64	10	74	

Table 2.14: Step time information of Triangular shot

Triangular							
Shot	Velocity	Frame	Add. Frame	Net Frame	Extra Frame	Input Frame	Chosen Frame
Small-Vert	95	24	32	56	10	66	66
	110	24	28	52	10	62	
	125	24	24	48	10	58	
Medium-Vert	85	32	36	68	10	78	78
	100	32	30	62	10	72	
	115	32	27	59	10	69	
Big-Vert	70	46	43	89	10	99	99
	85	46	36	82	10	92	
	100	46	30	76	10	86	
Small-Hor	125	22	24	46	10	56	56
	140	22	22	44	10	54	
	155	22	20	42	10	52	
Medium-Hor	110	26	28	54	10	64	64
	130	26	24	50	10	60	
	145	26	21	47	10	57	
Big-Hor	100	36	30	66	10	76	76
	120	38	25	63	10	73	
	140	38	22	60	10	70	

In many of mesh convergence studies, first simulation is initialized by relatively higher size of elements. These first simulations are not expected to provide accurate results. However, they can possibly point out the most stressed regions where user needs to do mesh refinement by replacing smaller elements instead of bigger elements in the most stressed regions.

Mesh refinement is the process of downsizing the elements both in stressed

Table 2.15: Step time information of Spherical shot

Spherical							
Shot	Velocity	Frame	Add. Frame	Net Frame	Extra Frame	Input Frame	Chosen Frame
Small	90	32	34	66	10	76	76
	110	31	28	59	10	69	
	130	30	24	54	10	64	
Medium	80	46	38	84	10	94	94
	95	44	32	76	10	86	
	110	43	28	71	10	81	
Big	70	50	43	93	10	103	103
	90	50	34	84	10	94	
	110	50	28	78	10	88	

regions and complete model. However as mesh sizes get smaller, number of meshes increase and this increases computational time and cost. In other words, a gain is gathered in the perspective of quality and accuracy of results but a loss is also received in the perspective of computational time and cost. Yet, mesh refinement must take place to get accurate results.

A mesh optimization shall take place in this kind of gain/loss situation. Because after some point of mesh refinement, mesh size will no longer influence the results where results will enter the zone of “mesh-independency”. The aim of all mesh convergence studies is to figure out this optimized point.

Bagherifard et al.[17] makes a similar study on reference model for shot-peening and evaluates an element size that puts the desired results into mesh-independent zone. A similar methodology to this paper is also applied in this thesis. First of all, a set of mesh sizes is listed. At this point, one of dimple regression models needs to be utilized. It is decided to use solely one regression model considering the fact that material properties do not vary between particle groups and sub-groups. For this purpose, spherical particle dimple regression model is used and a single dimple diameter is obtained. The reason for obtaining this dimple dimension is to have a reference for mesh sizes. Bagherifard et al. relates the smallest mesh sizes on substrate and all mesh sizes on shot particles to dimple dimension.

Initializing from this point, a set of mesh sizes is obtained as summarized in Table 2.16

Another series of single impact simulations shall now take place using the above-mentioned mesh sizes in the dense mesh zone of substrate and shot particle.

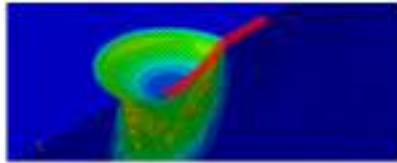
After completing these single impact simulations, 2 paths are created in

Table 2.16: Mesh sizes with their ratio to dimple dimension

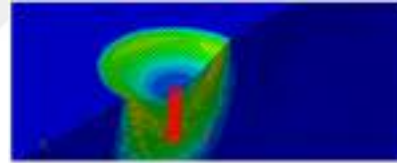
Dimple Diameter[mm]	Mesh/Dimple Diameter	Ratio	One Mesh Size[mm]	One Side of Mesh Square[mm]
0.547	0.1	10	0.055	2.4
	0.067	15	0.036	
	0.05	20	0.027	
	0.04	25	0.022	
	0.033	30	0.018	
	0.029	35	0.016	
	0.026	39	0.014	

Visualization module of FEA model. One path follows the nodes starting from the impact center and goes until the edge of the dense mesh zone, which is referred to as horizontal path. Another path is created starting again from the impact center but this time following the nodes vertically, penetrating through the substrate instance, this path is referred to as vertical. Results are mainly examined in 5 ways:

1. PEEQ in horizontal path
2. PEEQ in vertical path
3. U2 in horizontal path
4. U2 in vertical path
5. S22 in vertical path



(a) Horizontal path



(b) Vertical path

Figure 2.27: Representative directions of "Horizontal" and "Vertical" paths where points extracted from the deformed surface

Results for these categories are plotted through the paths mentioned. These plots can be examined in Figure 2.28,2.29,2.30,2.31and2.32.

As it is observed from Figure 2.29, the observed results come to converge at smallest mesh size/dimple diameter ratio of 1/25, more in precisely at convergence point, the smallest mesh size is 0.0219 mm. This value is accepted and used in the consecutive progress of the study as the smallest mesh size.

Having obtained dimple regression models, step time information and smallest mesh size information, Step 2.4 of Dimple Regression and Mesh Convergence terminates at this point.

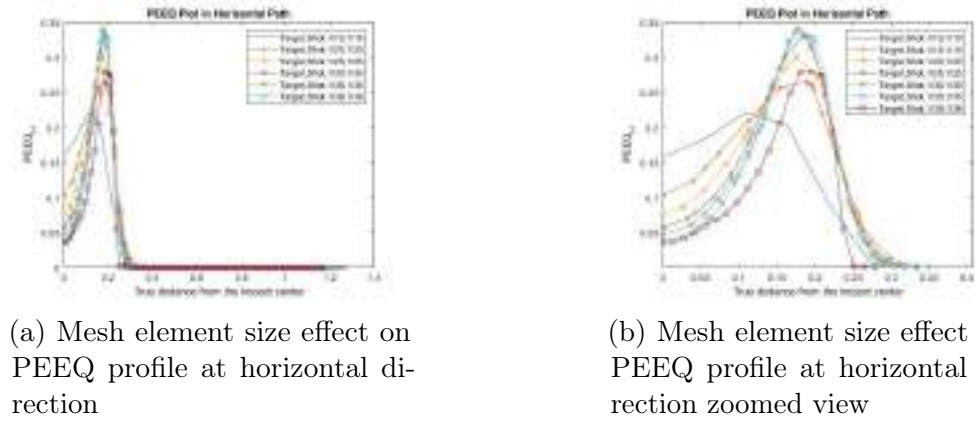


Figure 2.28: Convergence plots of PEEQ at horizontal direction

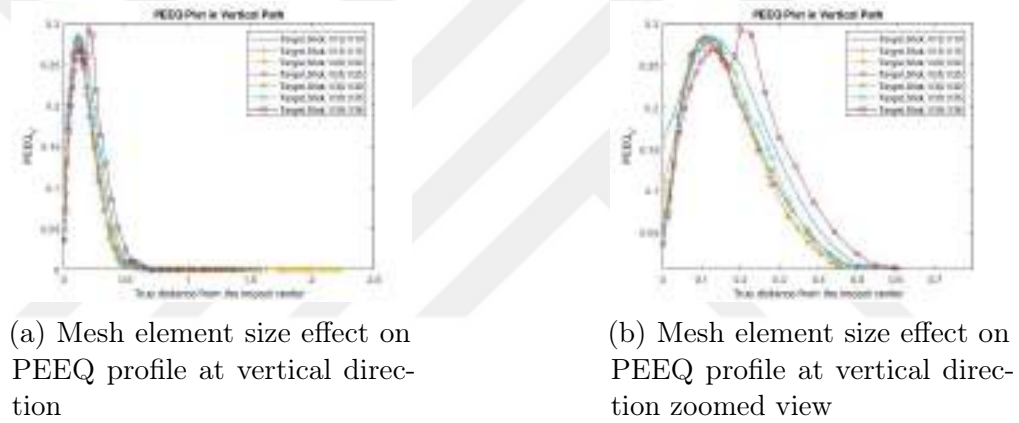


Figure 2.29: Convergence plots of PEEQ at vertical direction

2.5 Step 4: Multiple-Impact Simulation Model

Step 2.5 of Numerical Model Build-Up is the main step for running the simulation with multiple and consecutive impacts. With this perspective, first three steps can be considered as pre-process of this step where;

- Substrate and shots are characterized in Step 2.2
- Impact velocities are evaluated in Step 2.3
- Dimple models, step time and smallest mesh are determined in Step 2.4

Having obtained all these information, Step 2.5 must include FEA model with suitable coding and eventually shall lead to deformed substrate surface.

For this purpose, a series of processes must be organized. This organization shall not include solely FEA Model but also the arrangement steps for

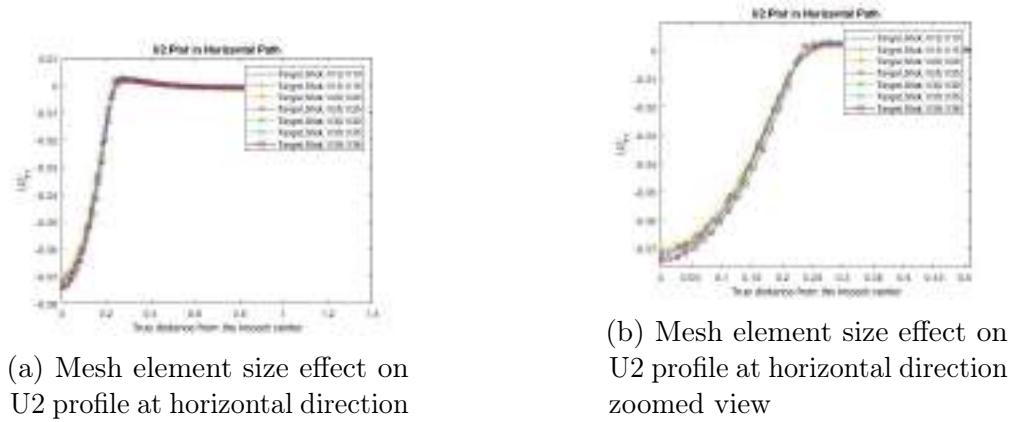


Figure 2.30: Convergence plots of U2 at horizontal direction

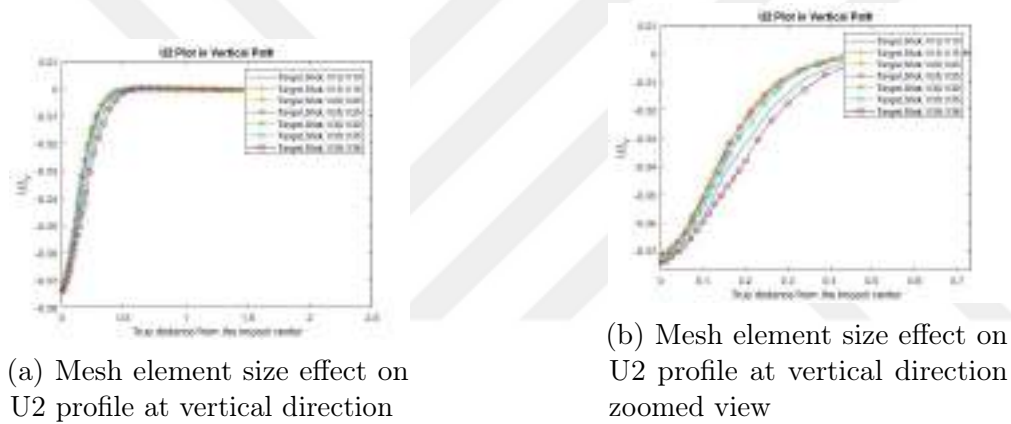


Figure 2.31: Convergence plots of U2 at vertical direction

inputting randomness and calling for the multiple impacts consecutively. This arrangement requires 3 main softwares to use listed below in Table 2.17 with their utilization purpose.

Table 2.17: Software used for building simulation

Software	Utilization
MATLAB	Randomness generation
PYTHON	Scripting for multi-impact simulation
ABAQUS	Dynamic/Explicit Simulation

Algorithm built for Step 2.5 can be examined in Figure2.33.

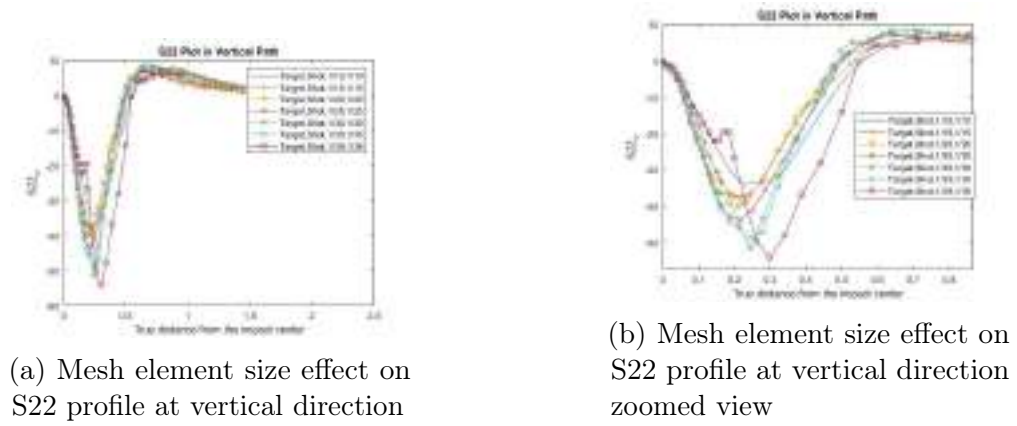


Figure 2.32: Convergence plots of S22 at vertical direction

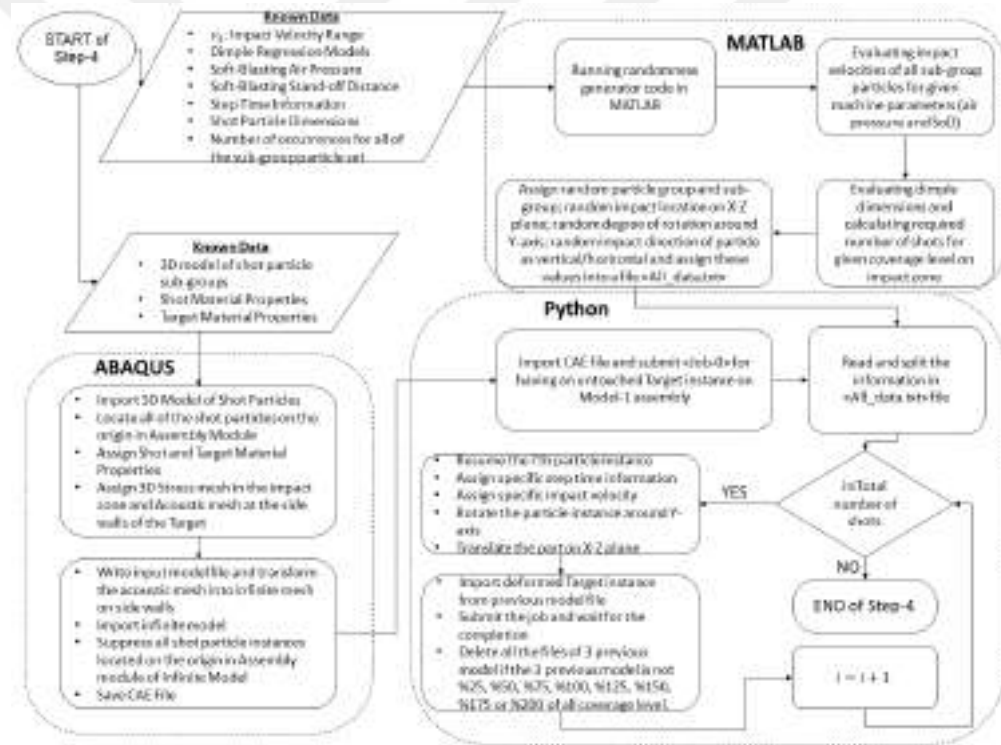


Figure 2.33: Algorithm of Numerical Model Step 4

This algorithm starts with two blocks of known data. One of these blocks provide information to MATLAB Random Generation phase which will then provide information to Python routine in the later step.

The other known data will work simultaneously and will give information

to ABAQUS while creating CAE model.

First block of known data will give the following information to MATLAB routine:

- Impact velocity range related with air pressure and SoD obtained from Step 2.3
- Dimple regression models that take shot dimensions and impact velocity as input and give dimple dimensions as output obtained from Step 2.4
- Soft-Blasting Air pressure range from real-life machinery and experimental plan
- Soft-Blasting SoD range from real-life machinery and experimental plan
- Step time information that will mainly be included in the Python script
- Shot particle dimensions obtained from Step 2.2
- Number of particles in each sub-group of particles obtained from Step 2.2

Other known data block progresses the following information to ABAQUS model:

- 3D models of all of the particle sub-groups obtained from Step 2.2
- Shot material properties obtained from Step 2.2
- Substrate material properties obtained from Step 2.2

These 3 softwares work in collaboration in the multiple impact (will also be referred to as multi-impact) environment. The processes in every routine will be explained in detail.

2.5.1 MATLAB Randomness Generator

The MATLAB code that is specifically written for Step 2.5 is enriched with the shot dimensions and velocity tables. These velocity tables are matching SoD and air pressure information that need to be input to MATLAB model and give the resulting impact velocity as output.

Having both shot dimensions and velocities, code is now able to figure out dimple sizes for all 21 impact sets. The code progresses dimple sizes for all of the impact sets. Then by using the percentages of particle sub-groups, it evaluates a representative dimple surface area for each group of the particle. Having obtained a representative dimple surface area for spherical, ellipsoidal, rectangular and triangular particle groups, code further utilizes the particle percentages between groups and calculates a single representative dimple surface area accounting for all of the particle groups. As impact set also varies the dimple shape and size, it must also

be included.

A decisive step is included into code for selecting between vertical or horizontal impact for particle sub-groups. A basic selection criterion is imported reflecting the following clauses:

- Chances of vertical/horizontal impact for ellipsoidal particles: 50% - 50%
- Chances of vertical/horizontal impact for rectangular particles: 50% - 50%
- Chances of vertical/horizontal impact for triangular particles: 25% - 75%

This basic decision is just modified in triangular particles as vertical impact means impact of base surface and horizontal impact means impact of one of three side faces. To reflect this weighting, chances are given as 75% for horizontal impact and 25% for vertical impact. For ellipsoidal and rectangular particles, chances are input as 50% both for vertical and horizontal impact.

Considering also these weightings, MATLAB evaluates a single representative dimple surface area. Yet the expectation is to have a different representative dimple surface area at different runs of the code since there is a random chance of picking the impact direction. This expectation is observed to be fulfilled at different runs since this single area information varies between these runs.

The reason for gathering this single area information is its utilization in coverage assessment.

Coverage Assessment

Bagherifard et al. [18] explains the coverage in this paper and also in some other papers of the authors. This paper specifically analyses the coverage.

Coverage is mainly the ratio of plastically deformed area in the region to complete area of region [59]. It is one of the most important parameters since it is the starting point of the model. MATLAB code is initialized out of evaluation of number of required shot particle impacts for a given coverage. As explained by Bagherifard et al. [18], Avrami equation 2.10 is one of the most commonly used equations in this perspective [30].

$$Cov\% = 100 [1 - e^{-A_r}] \quad (2.10)$$

This formulation functions over a single area information rather than having a range or series of values. That is the main reason behind identifying a

single area information characterizing all of the particles based on their occurrences in the complete set.

The complete impact region shall also be defined at this step. As will also be explained in Step 2.6, Post-Processing, experiments will follow the standard ISO-4288 where different sets of measuring lengths are applied. The selected set for both the model and experiments have 1.25 mm of measuring length. Thus, one side of square of impact zone is input as 1.25 mm.

In this configurations, MATLAB code is run few times to see the variation in the detection of number of shots on 1.25 mm x 1.25 mm impact square. The mean of this number is found out to be 15 while also giving results between 13 and 17. So, the number of required Alumina shot particle impact on 1.25 mm x 1.25 mm square can be summarized as 15 ± 2

Once MATLAB code gathers the information of required shot number, the next process is to locate random shape and size shot particles randomly on impact square while also randomly picking their impact direction as vertical or horizontal and randomly picking their degree of rotation around Y axis. To summarize all these factors, the following list of the randomness elements can be examined:

- Random selection of particle group (shape)
- Random selection of particle sub-group (size)
- Random impact direction (vertical or horizontal)
- Random degree of rotation around Y axis
- Random translation on X and Z axis

Code firstly makes and assigns all the randomness criterions for the first impacting particle. Then it inputs the random factors into corresponding tables. The information on these randomness data for the first particle become the first element for each factor table.

Then code initializes a while loop in which it starts assigning all the randomness starting from the second particle and lasting until the last number of particle which was previously evaluated within given specific coverage level. That's how coverage assessment initializes the code.

Code does exactly the same steps inside the while loop for each particle as it does while assigning the first particle except one difference. That difference can be referred to as "Avoiding Overlaps".

Avoiding Overlaps

MATLAB Code must ensure that overlaps do not occur while locating the particles on the impact zone or occurs at possibly the lowest degree. For this purpose, a code is input in the reference FEA model for shot peening process family which is updated based on the concept of this thesis. Inside the while loop, MATLAB assigns the X and Z locations of the center point of the particle. Reference model evaluates the distance between this new point to all other points that are previously considered valid and input in the set and makes a decision based on a threshold. If all of the distance values are greater than this threshold, then this point is accepted as a new point and code progresses with impacting a particle having that point as the center.

Selection of that threshold is done based on the dimple diameter. As there are only spherical particles in the reference model, dimple shape is solely spherical. The threshold is accepted as $1/3$ of dimple diameter. In other words, the required distance between centers of valid impacting particles is considered to be at least $1/3$ of the characteristic dimension that their dimple would create.

Having the same perspective, the distance parameter needed to reflect the contribution of other geometrical shapes in the concept of this thesis. As reference model took spherical dimple diameter as the characteristic dimension for this purpose, this new model takes again the diameter for spherical dimples; average of minor and major diameter for ellipsoidal dimples; diagonal for rectangular dimples and height for triangular dimples as the characteristic dimension.

Taking these dimensions for all sub-groups of particles and obtaining their average gave one single characteristic dimple dimension just like the concept of one single surface area information. Reference model divides characteristic dimple dimension and divides it by 3. Same operation is also followed here. The required distance is established as $1/3$ of single characteristic dimple dimension as in figure 2.34.

This way, possible overlaps between different geometries are minimized.

After assigning all of the random factors for complete set of particles, while loop reaches and evaluates the last particle and then terminates. All of the randomness factors are now listed in their corresponding tables.

Next step is to gather all these information into one single table and then exporting this table as .txt file and this is how the code progresses.

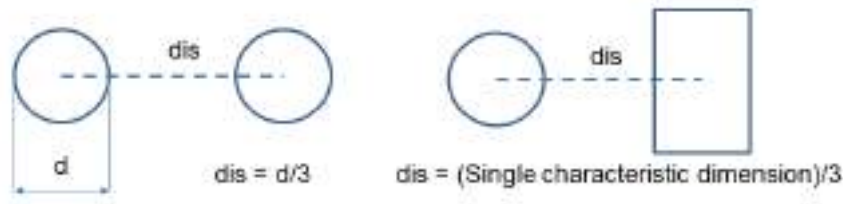


Figure 2.34: Representative distance evaluation for spherical shot(Left) and for different geometries(Right)

The image shows a Notepad window titled 'All_data.txt - Notepad'. The window contains a list of data entries, each consisting of two numerical values, a particle description, and two more numerical values. The status bar at the bottom indicates 'Ln 13, Col 43', '100%', 'Windows (CRLF)', and 'UTF-8'.

```

File Edit Format View Help
0.35466 0.030283 rect_med horizontal 158 137.1
0.16765 0.33578 tri_med horizontal 323 139.2
-0.3784 0.23459 tri_med horizontal 119 139.2
0.5565 -0.35923 tri_small horizontal 190 153
-0.37718 -0.46718 tri_med horizontal 62 139.2
-0.026276 -0.40377 sp_small vertical 0 120.6
-0.13565 -0.1493 sp_big vertical 0 98.07
0.17795 -0.62181 sp_small vertical 0 120.6
0.045677 0.066093 ell_small vertical 113 109.5
-0.56361 -0.15116 rect_small vertical 3 126
0.41921 0.51196 sp_small vertical 0 120.6
-0.52591 0.46884 tri_small horizontal 180 153
-0.17062 0.39013 sp_small vertical 0 120.6

```

Figure 2.35: All_data.txt file

A representative image of All_data.txt file can be seen in Figure2.35 where first two variables represent translations on X and Z axis in mm, third variable represent group and sub-group of the particle, fourth variable represents impact direction, fifth variable represents degree of rotation around Y axis and the last variable represents the particle impact velocity.

MATLAB code plots particle dimples on impact zone before it terminates. Different outputs of the code in different runs can be visually examined in Figure 2.36. There are 2 squares that can be observed one being red and one being blue. Blue square represents impact zone with one side being equal to 1.25 mm and red square represents the dense mesh zone in ABAQUS. Dense mesh zone completely contains smallest meshes. In other words, regions inside the red and blue square is composed of same size of meshes. The reason for existence of red square in these plots is to ensure that all particles impact on smallest meshes. Otherwise, simulations are observed to terminate with error after some number of impacts. Thus, the user of the code must consider the data set output of MATLAB only if all particles are completely inside the red square.

A basic solution would be enlarging the area of red square and thus dense mesh zone in ABAQUS. However, this would also greatly increase the computational time. An optimum value for one side of red-square is found out to be 2.4 mm and CAE model is arranged accordingly.

Having obtained required data for Python routine, MATLAB routine ends here.

2.5.2 ABAQUS FEA Model

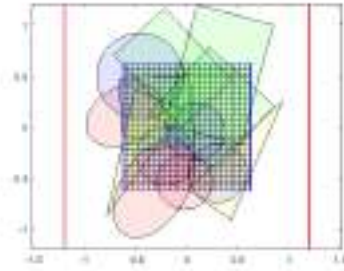
CAE model is planned to have a series of single instances imported. The substrate instance that will represent the substrate material is highly referenced by previous shot-peening process family numerical simulations while modifying some dimensions on it like dense mesh square and some mesh partition arrangements.

Shot particles are all imported from Catia V5 R19 after having been obtained at the end of Step 2.2. In fact, total of 21 shot instances are imported to account for all impact sets. As an example, ellipsoidal medium particle is imported twice for vertical and horizontal impact.

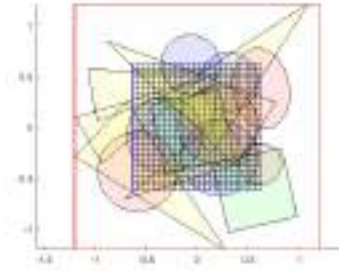
All of these particles are then located on the origin with corresponding directions by assigning position constraints. A representative visual can be seen in Figure 2.37 for all the particles being located on the origin.

Shot and substrate material properties for Alumina and PC are input in the Property module. These properties have been obtained in Step 2.2.

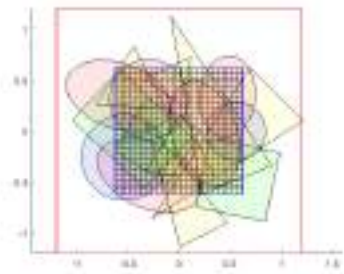
An important aspect shall be mentioned in Property module at this point. As will be explained later in this step, the created CAE model will then be transformed into Infinite model with the details explained below. However,



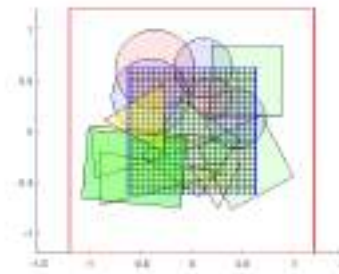
(a) Output with machine parameter of 6Bar and SoD of 150mm



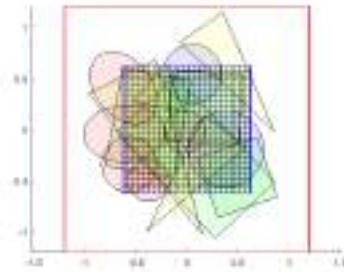
(b) Output with machine parameter of 6Bar and SoD of 150mm



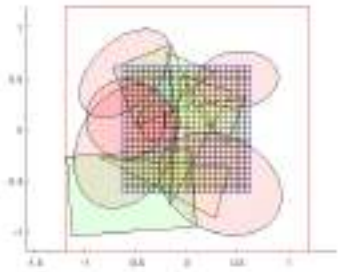
(c) Output with machine parameter of 6Bar and SoD of 150mm



(d) Output with machine parameter of 6Bar and SoD of 150mm



(e) Output with machine parameter of 6Bar and SoD of 150mm



(f) Output with machine parameter of 6Bar and SoD of 150mm

Figure 2.36: MATLAB output visuals

a critical step needs to be done in here, Property module. The first model (referred to as “Acoustic Model”) will have no Load information for the velocity but the second model (referred to as “Infinite Model”) will apply the impacting velocities to the particles. As infinite model will mainly consist of orphan mesh, the processes have limitations in this model. The velocity loading operation requires a naming process in Acoustic Model.

For this purpose, all of the shot particles are assigned a region set while

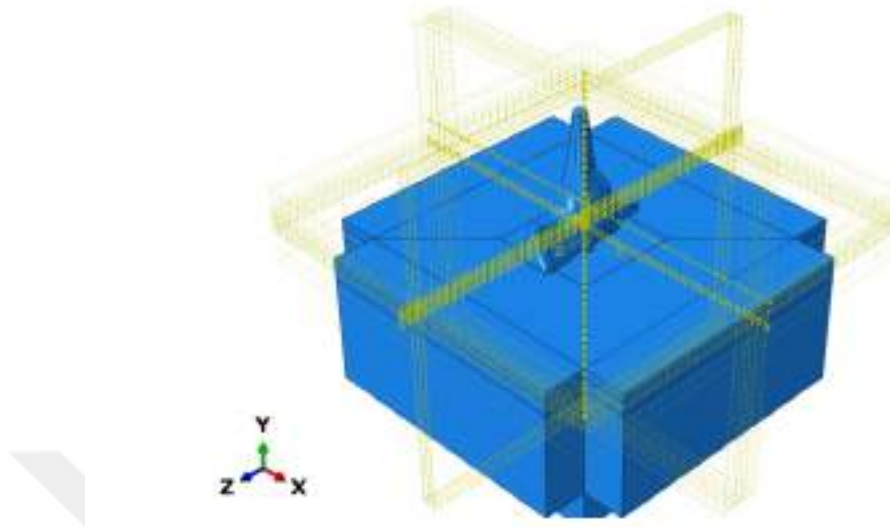


Figure 2.37: Assembly model

being section-assigned for their material properties. This way, it is possible to call these regions by their names in later Python script and assign a velocity loading.

In Step module, Dynamic/Explicit step is created but as previously explained, step time information will be varied at each iteration of Python routine influenced by particle shape, size and velocity.

Five field outputs are requested at each time increment of 1E-07 s. These field output parameters and their explanations are listed in Table 2.18

Table 2.18: Field outputs with their explanations (CSTRESS, PEEQ, S, U, V)

CSTRESS	Contact Stress
PEEQ	Equivalent plastic strain
S	Stress component and invariants
U	Translation and Rotation
V	Translation and Rotational velocities

Interaction is assigned as general contact with friction coefficient of 0.2 [19], [39]. As already said, no load is applied in Acoustic Model.

No boundary conditions are assigned to substrate but side walls are planned to be represented by half infinite meshes [1], [60] . For this purpose, side walls that are shown with color yellow in Figure 2.38 are assigned Acoustic mesh (AC3D8) in the Acoustic model and then transformed to Infinite model at later step.

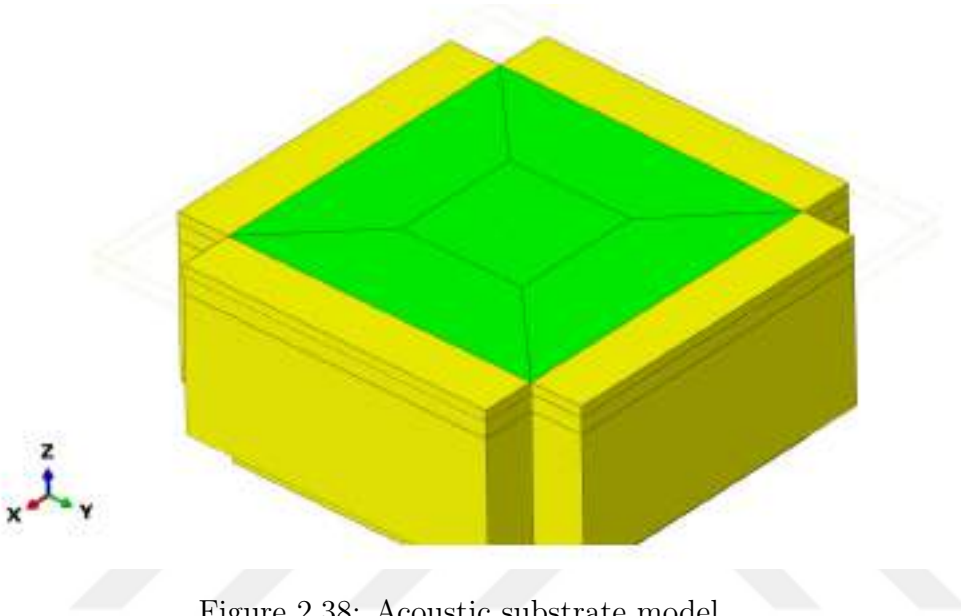


Figure 2.38: Acoustic substrate model

The other regions of substrate instance including the dense mesh zone is assigned 3D stress element with reduced integration and hourglass control. As they are 8-node, linear brick elements, element type is C3D8R. All of the meshes of shot instances are also 3D stress elements and they are also meshed with structured-Hex meshes except for the triangular particles which have been meshed with Tet meshes since meshing the Triangular Pyramid particles with given fillets were complex with Hex meshes. Mesh types and total element number for all particles and substrate is shown in Table 2.19

Once meshing is complete, input model file is written and saved to work directory in Job module. Then, by modifying AC3D8 to CIN3D8, in the input text file of this Acoustic model and then importing that model into ABAQUS back again, Infinite model is created.

Infinite model is composed of orphan mesh having half infinite meshes at side walls as planned.

Python script is planned to run over this Infinite model, so a further

Table 2.19: Summarizes element number information for all shot particle instances and substrate instance

Part	Element Type	Number of Element
Substrate	C3D8R	1007160
	AC3D8	42460
Spherical Small	C3D8R	31616
Spherical Medium	C3D8R	85536
Spherical Big	C3D8R	148896
Ellipsoidal Small	C3D8R	23328
Ellipsoidal Medium	C3D8R	68952
Ellipsoidal Big	C3D8R	168112
Rectangular Small	C3D8R	29952
Rectangular Medium	C3D8R	53946
Rectangular Big	C3D8R	96705
Triangular Small	C3D10M	39737
Triangular Medium	C3D10M	43790
Triangular Big	C3D10M	97116

arrangement needs to be done before proceeding with saving CAE file and ongoing with Python routine. All of the shot particle instances that have been located exactly on origin above substrate in Acoustic model need to be suppressed in the Assembly module of Infinite model. This way, Python routine will only resume the specific instance in current model and submit the job accordingly.

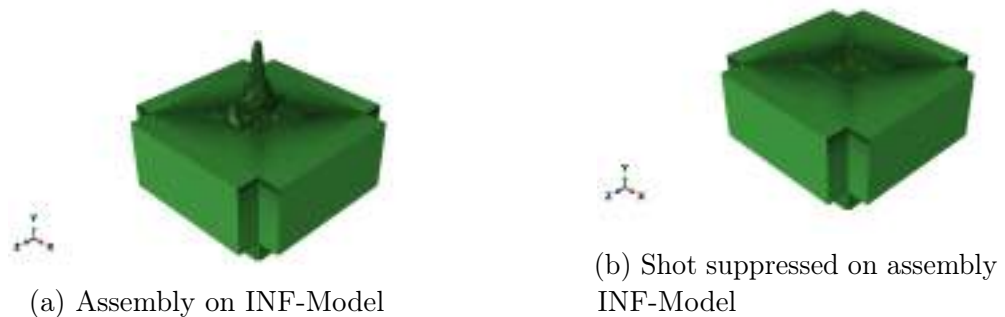


Figure 2.39: Transition from assembly to suppressed INF-Model

After suppressing the shot instances as shown in Figure 2.39, only substrate remains in Assembly module of Infinite model. Having reached to this step, CAE file can now be saved and exited.

2.5.3 PYTHON Multiple Impact Script

As can be observed from Figure 2.33, Python routine has inputs both from MATLAB and ABAQUS.

User must provide the inputs of initial shot number, maximum shot number and number of CPU's to use during the simulation to Python routine script. As initial shot number is an input, this system is able to start again the simulations from a point where it has been stopped at.

Python script is initialized with opening .cae file that was saved in ABAQUS phase. Then it copies the infinite model to a new model "Model-0" which shall act as a reference for consecutive impact sequences. In other words, Python script is entitled to deliver deformed substrate instance from previous job to current job as will be explained in the latest section of the script. However, when the first particle is there to impact on substrate, there shall be a substrate inside an odb file with name "Job-0" upon which "Model-1" can obtain the untouched substrate instance from.

Code copies Infinite model to "Model-0" and submits a job without resuming any shot particle instance. As there is no interaction in this job, step time is given with a small amount for the simulation not to occupy high computational time.

Once "Job-0" is completed, script reads the data in "All_data.txt" file obtained from MATLAB and splits the data inside correspondingly. Now having obtained all the required randomness information that were previously evaluated in MATLAB, Python script is ready to start consecutive impact sequences.

Script has 21 blocks for 21 impact sets. These blocks are called with if blocks being caught by their name which is utilized to characterize both group and sub-group of the shot particle. For instance;

- sp_small means Particle Group: Spherical and Particle Sub-Group: Small
- ell_med means Particle Group: Ellipsoidal and Particle Sub-Group: Medium

As impact sets are also characterized by impact direction, a further if

block is utilized to distinguish the impact direction whether it is vertical or horizontal.

After Python identifies the impact set, it firstly assigns the step time based on Table 2.12 , Table 2.13 , Table 2.14 , Table 2.15.

Then it resumes the specific part instance that is being caught by the name of the impact set. Having done so, that specific shot particle instance is now back again at the origin above the substrate.

Then script assigns the impact velocity to complete region of the shot particle instance. As it is mentioned before, region sets are utilized specifically for this purpose.

Later step is to rotate the particle around global Y-axis as it is still at the origin. Once rotation is complete, translation takes place. Translation on X and Z axis are taken from “All_data.txt” file. Y-axis translation is manually input at this step to avoid any kind of initial contact situation between shot and substrate. To fulfill this requirement, Y-axis translation is input as 0.3 mm at this step. All steps are shown in Figure 2.40

Having completed the Translation phase, block terminates.

Once script ensured the position and direction of particle, it calls for the deformed substrate instance from the previous Job odb file as a Predefined Field. As there is now both deformed substrate and new impacting shot particle, current job is ready to be submitted and this is how script progresses.

Script waits for the completion of the current job and once it is complete, it deletes all of the Job files of 3 previous model if that model is not one of the following:

- 25%
- 50%
- 75%
- 100%
- 125% (for models going beyond 100% coverage)
- 150% (for models going beyond 100% coverage)
- 175% (for models going beyond 100% coverage)
- 200% (for models going beyond 100% coverage)

of total number of shots. The reason behind this is to limit the free space occupation in the computer as the job files can be very space-consuming.

As Python script ends here, the only remaining step is to open ABAQUS and run this Python script located together in a folder with “All_data.txt”

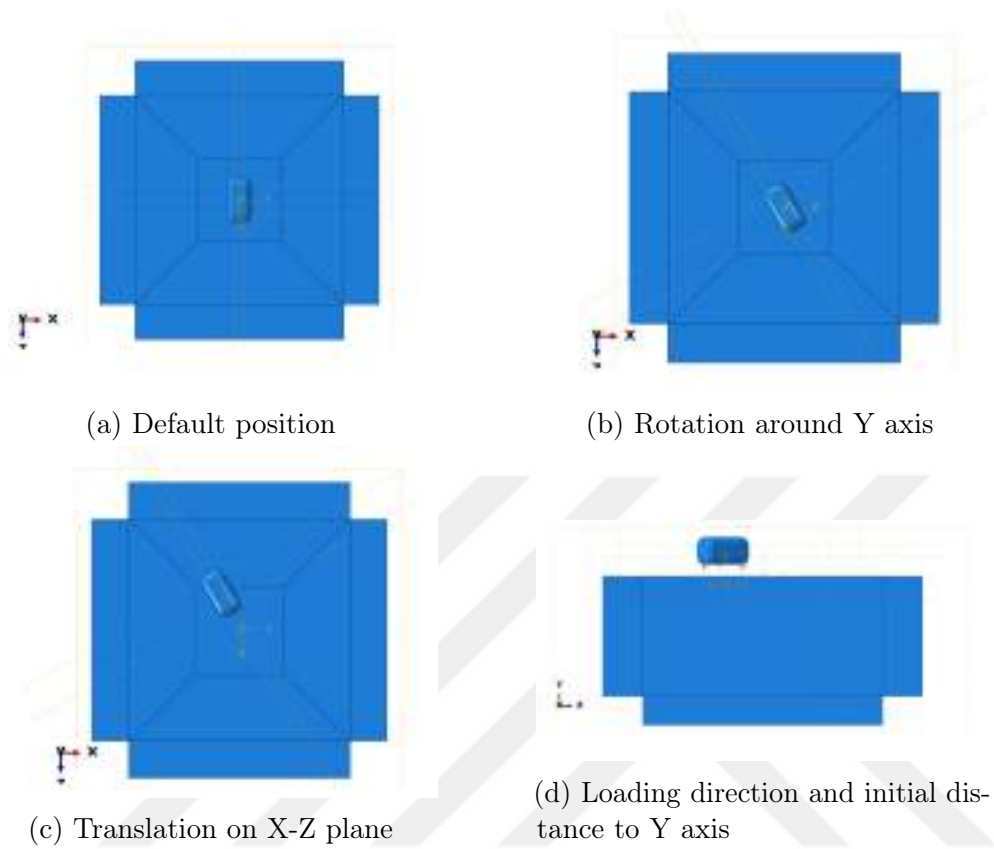


Figure 2.40: Steps done on python script in sequence order

file from MATLAB phase and .cae and .jnl files from ABAQUS phase. This is how Step 2.5 terminates.

2.6 Step 5: Post-Processing

In Figure 2.41, the algorithm built for Step 2.6 can be seen.

Once Multi-Impact Simulation is complete, next step is to arrange the required operations to examine surface morphology and evaluate surface roughness parameters upon which the experimental validation will take place.

Figure 2.42 shows a representative image of final deformed substrate surface in one of the simulation sets that have been computed. All the dimples that have been created by consecutive shot particles can be seen on substrate surface.

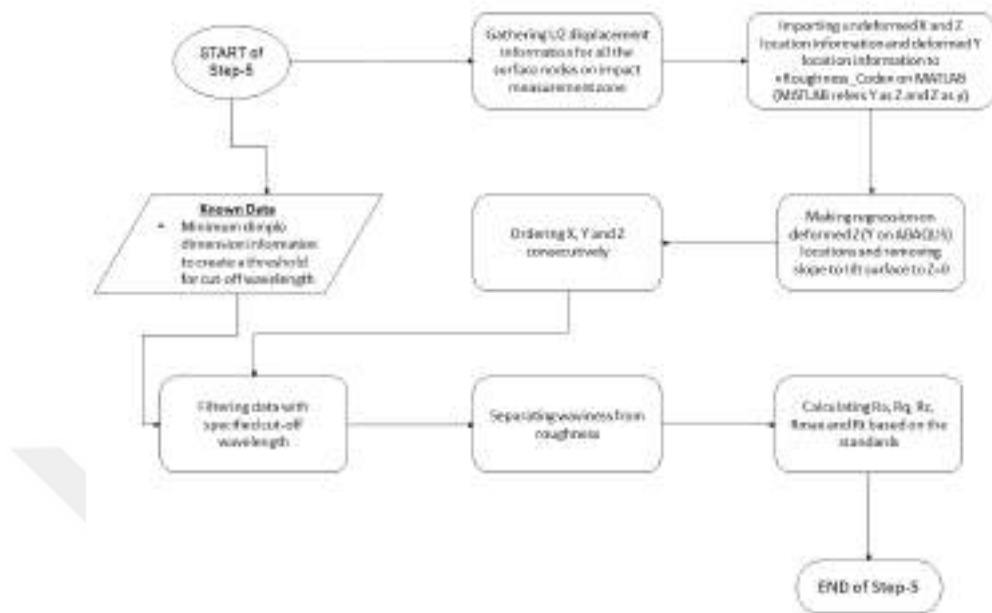


Figure 2.41: Algorithm of Numerical Model Step 2.6

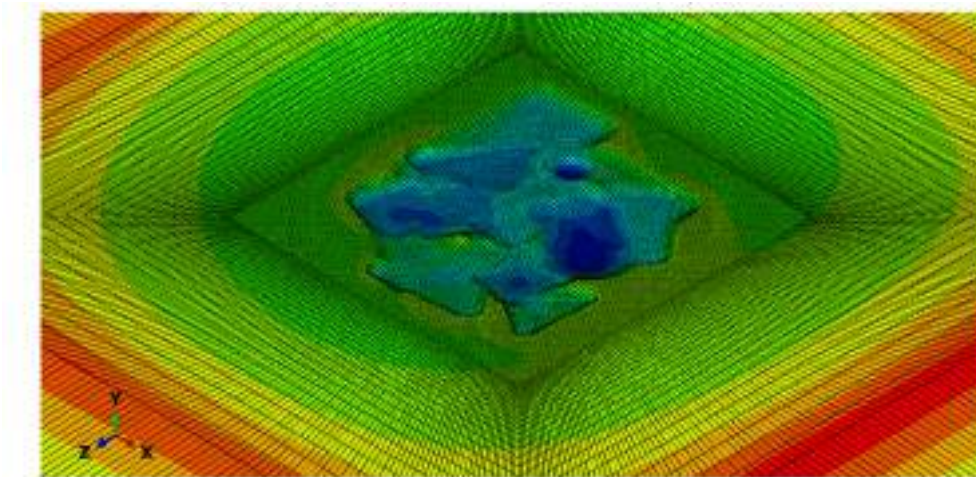


Figure 2.42: Result of one simulation

At this point, an element removal process shall take place to trim the unnecessary elements from the substrate instance. As can be remembered

from Figure 2.36, it is mentioned that substrate will have a dense mesh zone where the meshes will have the smallest size inside the red square whereas the impact and measurement zone is only the blue square. Figure 2.36 shows that not all the smallest meshes are impacted as mentioned. Thus, substrate will be trimmed in such a way that it will consist of only the impact and measurement zone nodes and elements at the top surface.

Once trimming operations take place, substrate becomes the visual as in Figure 2.43.

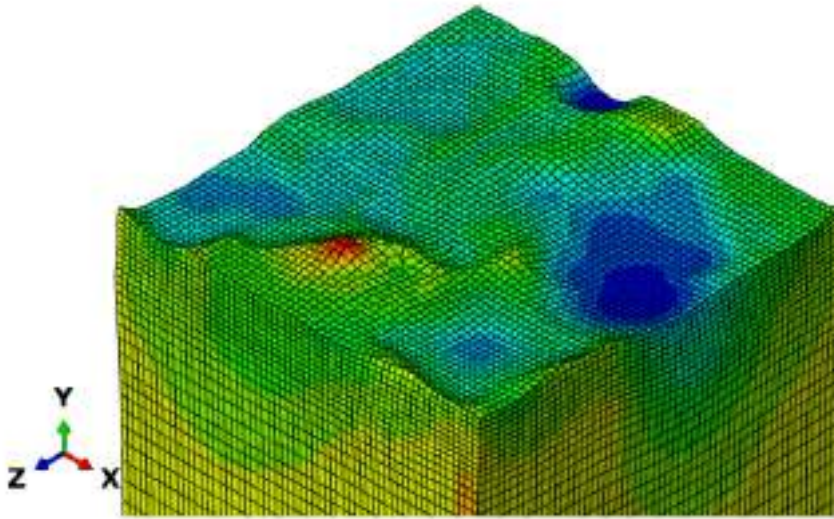
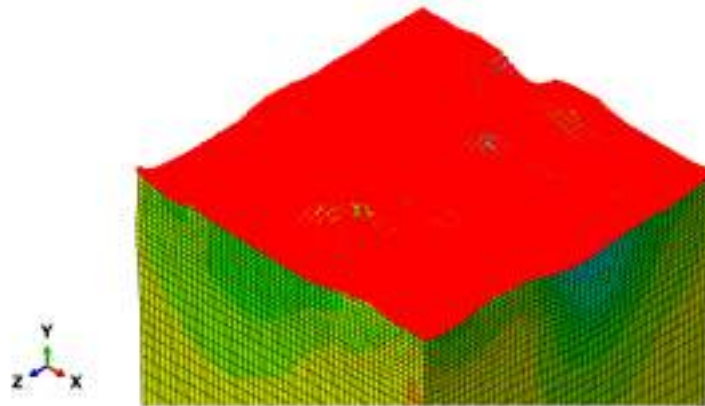
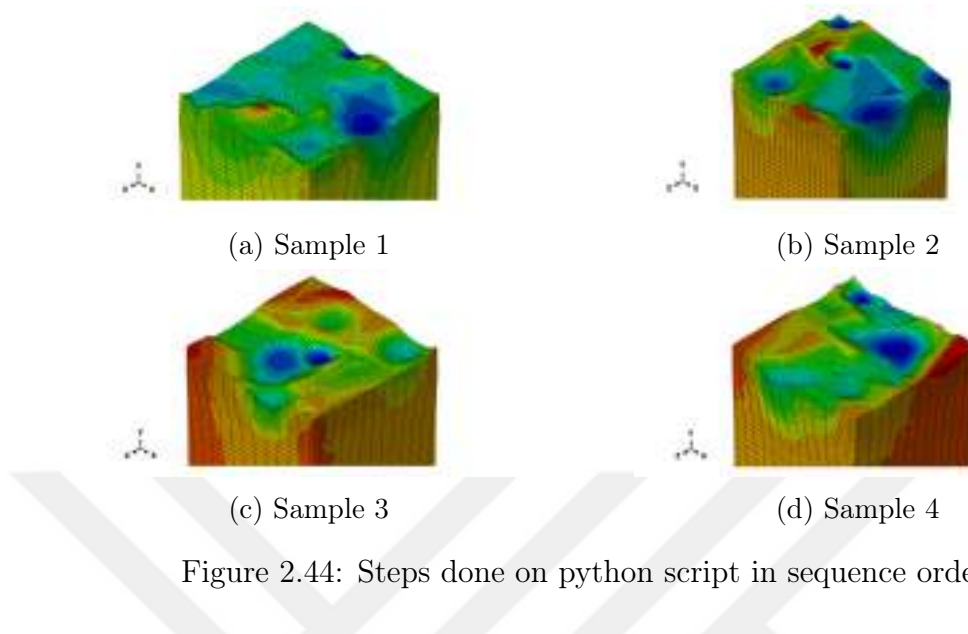


Figure 2.43: Result of one simulation trimmed to take data point

As the one side of the impact and measurement square zone is 1.25 mm, the region that is seen in ABAQUS Visualization module in Figure 2.43, is also a square with having a side dimension equal to 1.25 mm.

Once the final surface morphology is obtained in ABAQUS, A Display Group is created by selecting the nodes. The nodes are selected by calling them on angle and selecting them all in once easily. Figure 2.45 shows the selected nodes in the upper surface.

As specified, one side of the impact square is 1.25 mm and size of the smallest mesh is 0.0219 mm. Considering this, following equations take place.



$1.25 \text{ mm} / 0.0219 \text{ mm} = 57.08$ elements rounding up to the 58 elements shall be placed alongside the side of the impact zone. This means that there are 58 elements on one side of the square. So, there shall be 59 nodes on one side of the square. To check the accuracy of the Display Group selection, this information can be used. As there are 59 nodes on one side, Display Group must select $59^2=3481$ nodes and this is used as a verification tool while creating Display Groups in all simulation sets.

Plotting U2 values on the contour and getting Probe values for all the nodes in the Display Group, a file is obtained that contains both original

and deformed coordinates of all of the nodes in the set.

Next step is to go back to MATLAB for surface roughness parameters extraction. This MATLAB routine for roughness extraction mainly separates waviness (low-frequency features of the profile) and roughness (high-frequency features of the profile) and works in the same methodology used by Khajehmirza et al [31]. One basic issue should be mentioned here. MATLAB has a rotated coordinate system with regards to ABAQUS. X axis is same but Y axis becomes Z axis and Z axis becomes Y axis while going from ABAQUS to MATLAB for Post-Processing. To summarize, following phrases can be analysed.

- ABAQUS: Impact surface plane: XZ and Impact direction: Y axis
- MATLAB: Impact surface plane: XY and Impact direction: Z axis

MATLAB Code for Roughness extraction requires three sets of data. Undeformed X and Y coordinates and deformed Z coordinates. By matching the right axis between softwares, the required data set is input to MATLAB.

As explained in Chapter (ref-surface morphology chapter in Introduction), a filtering must take place to extract roughness out of primary profile as primary profile consists of both Waviness and Roughness. The concept of this thesis is to examine Roughness as one of the motivations is to provide a model ready to include wettability phenomenon in the future and wettability is mainly influenced by Roughness.

Before going with filtering, MATLAB code makes three important operations on the data. It firstly makes a regression to tilt the surface up to $Z=0$. In other words, the mean line of the deformed surface extracted from ABAQUS is not 0 but another value that is unknown. This operation is done to get the surface to mean line of $Z=0$ and locate it onto XY plane.

Next process is to order the data on X and Y axis consecutively. This is mainly done since the ordering of ABAQUS is not known when the data is imported to MATLAB.

And as a last step before filtering, MATLAB smooths the data with a series of operations including linspace command. As it can be remembered, there were 59 nodes on one side of the impact square. MATLAB takes this value to a higher value by a smoothening operation while keeping the same behavior of the data with the motivation of better and improved characterization of the surface morphology. In the concept of this thesis, smoothening points number is taken as 1000.

Before proceeding with the filtering, MATLAB plots the surface in a 3D

view as can be seen in Figure 2.46.

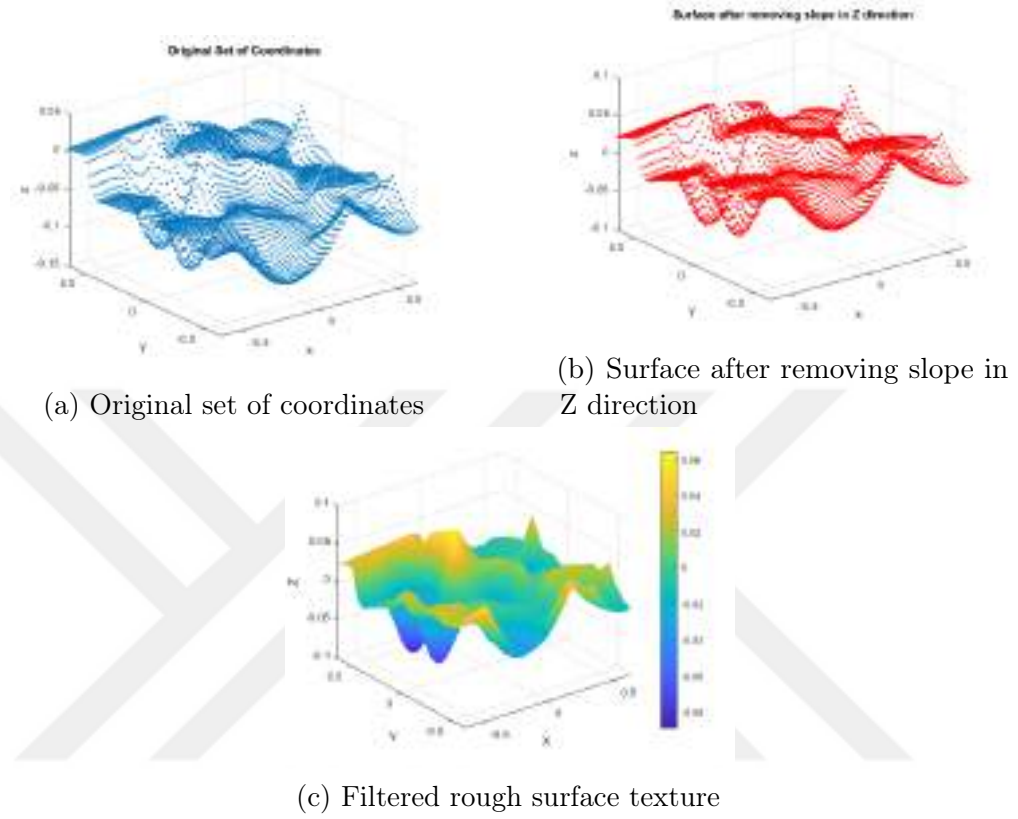


Figure 2.46: Post processing visual results

Then a low-pass Gaussian filter is applied as shown in Equation 2.11 where $\alpha = \sqrt{\ln(2)/\pi}$ and λ_{xc} and λ_{yc} are the cut off wavelengths used to filter the data in the corresponding directions.

$$S(x, y) = \frac{1}{a^2 \lambda_{xc} \lambda_{yc}} \exp \left[- \left[\pi \left(\frac{x}{a \lambda_{xc}} \right)^2 + \pi \left(\frac{y}{a \lambda_{yc}} \right)^2 \right] \right] \quad (2.11)$$

This lowpass Gaussian filter is a 3D filter and it works in both directions of X and Y. The selection of cut-off wavelengths must comply with ISO-4288. Cut-off wavelength and evaluation length selection with regards to ISO-4288 is summarized in Figure 2.47.

A decisive step must be taken into account here to choose the cut-off wavelength. For this purpose, a better approach to cut-off wavelength function must be done.

Cut-off raccomandati – Norma ISO 4288-1997				
Profili Periodici	Profili NON Periodici		Cut-off	Lunghezza di Campionamento / Lunghezza di Valutazione
S_m [mm]	R_z [μm]	R_a [μm]	λ_c [mm]	λ_c/L [mm]/[mm]
$0,013 < S_m \leq 0,04$	$(0,025) < R_z \leq 0,1$	$(0,006) < R_a \leq 0,02$	0,08	0,08/0,4
$0,04 < S_m \leq 0,13$	$0,1 < R_z \leq 0,5$	$0,02 < R_a \leq 0,1$	0,25	0,25/1,25
$0,13 < S_m \leq 0,4$	$0,5 < R_z \leq 10$	$0,1 < R_a \leq 2$	0,8	0,8/4
$0,4 < S_m \leq 1,3$	$10 < R_z \leq 50$	$2 < R_a \leq 10$	2,5	2,5/12,5
$1,3 < S_m \leq 4$	$50 < R_z \leq 200$	$10 < R_a \leq 80$	8	8/40

Figure 2.47: ISO-4288 standart table

What cut-off wavelength mainly does is to trim the data in space domain based on a frequency threshold. In other words, inputting a cut-off wavelength of a value as x (mm) would let the low-pass filter to filter the features on the profile with higher characteristic dimension than x and thus lower frequency.

MATLAB code progresses with convolution step and obtains waviness data after convolution step. As the main motivation is to gather roughness, evaluated waviness data must be subtracted from the main profile data to obtain roughness and that's how the code processes.

As already explained, a rightful selection of cut-off wavelength is crucial. When the methodology of the sand-blasting and its relation with surface roughness construction is considered, it shall be mentioned that the longest wavelength located on the profile should not have a value higher than the dimple diameter as also stated by Bagherifard et al [16]. As this study contains a series of dimple dimensions, the smallest dimple dimension should be considered here. When the dimple dimensions are examined together with ISO-4288 cut-off selection table, 0.25 mm is chosen as cut-off wavelength as there are dimples with characteristic dimensions lower than 0.8 mm which is just the next higher cut-off wavelength value in ISO-4288. But there are no dimple characteristic dimensions lower than 0.25 mm.

As the filter is used and firstly waviness and then roughness datas are

gathered, next step is to obtain surface roughness parameters. The selected surface roughness parameters to use in Experimental Validation chapter are as the following:

- R_a : Arithmetical mean of absolute values of entire roughness data over evaluation length
- R_q : Root mean square of entire roughness data over evaluation length
- R_t : The difference between highest peak and lowest valley of the roughness profile over evaluation length
- R_z : The average of 5 peak-valley distances over evaluation length
- R_{max} : Maximum of the 5 peak-valley distances over evaluation length

To better explain R_z and R_{max} , sampling length concept must be highlighted. Evaluation length is segmented into 5 pieces each having a length of 0.25 mm. In each of these segments, a local R_t (now being R_{ti}) is evaluated. R_z is happened to be mean of these 5 values where R_{max} happens to be their maximum value.

The explanations of these parameters can also be examined in Figure 2.48.

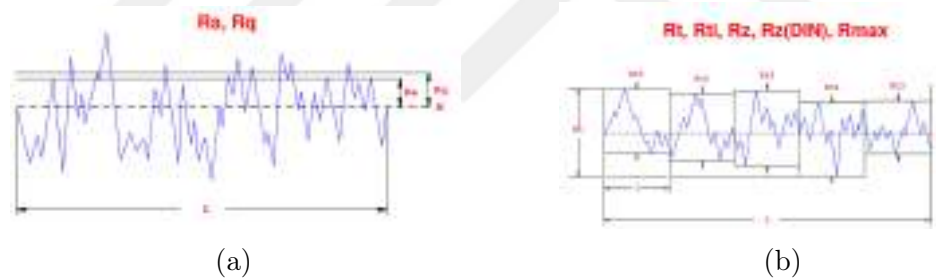


Figure 2.48: Surface Roughness parameters [61]

As already mentioned, smoothening points number is taken as 1000 in the utilization of MATLAB code for the progress of this thesis. This means that, MATLAB will calculate all these surface roughness parameters 1000 times through a direction as shown in Figure 2.49. As this is a 3D approach model and roughness needs to be examined in two different directions, MATLAB code will evaluate roughness parameters for 1000 times considering the other direction as well. This will give a variety of surface roughness parameters. For experimental validation phase, both mean of these values and their variety will be taken into account.

Results of the one i'th segment through X and Y direction can be seen in Figure 2.50

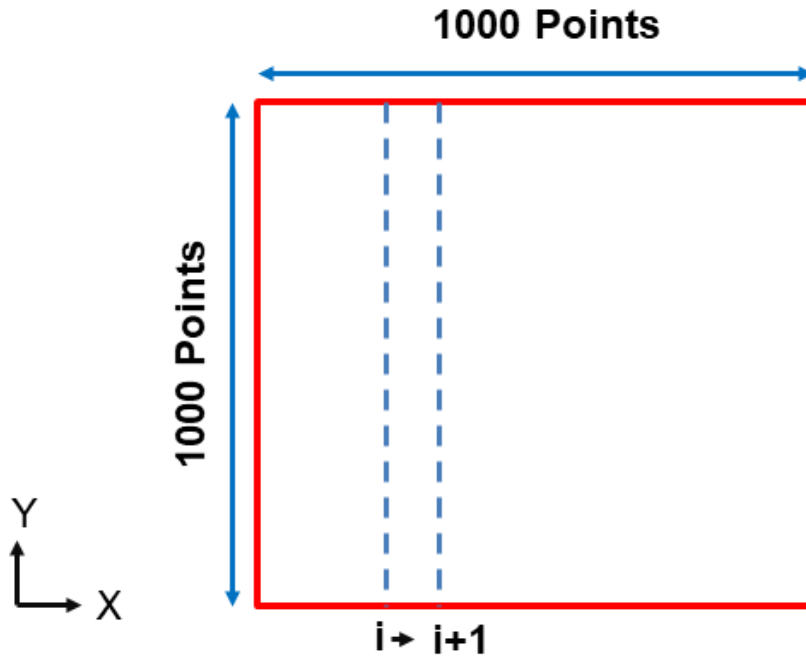
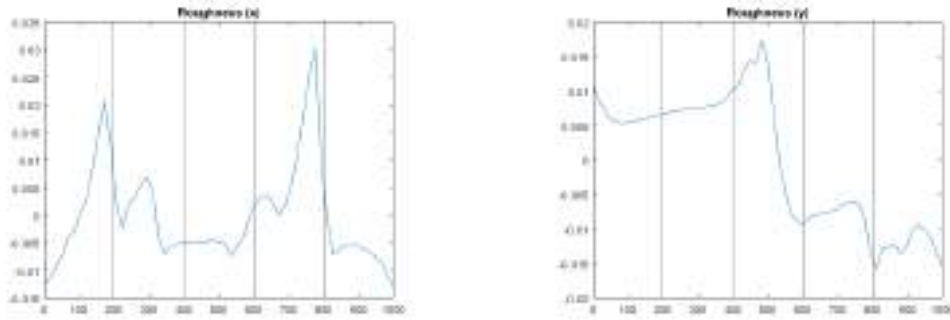


Figure 2.49: Roughness extraction methodology

Figure 2.50: Roughness profile at any i 'th segment

Having calculated required surface roughness parameters, Step 2.6 of Numerical Model Build-Up and thus the complete construction procedure terminates here. Next progress in the entire thesis is to conduct the related experiments and validate the model by comparing the surface roughness parameters evaluated in this Step 2.6 with experimental findings.

2.7 Model Enhancements

Extension Model

The simulations that are run by the so-far mentioned arrangement give promising results but several possible enhancements on the built model are noticed.

It is noted that the penetration level of ellipsoidal and spherical shot particles are considerably higher than the penetration level of rectangular and triangular shot particles. The main reasoning behind this is the initial contact situation between the shot particle and the substrate.

Spherical and ellipsoidal particles by their nature have a point contact with the substrate. However, rectangular and triangular parts are considered to have flat surfaces which creates a face contact with the substrate at the initial condition. As the contact stress is dispersed to a surface rather than a point, this effect makes the rectangular and triangular particles to penetrate less into the substrate. When SEM images of the Alumina are considered, the high irregularity also makes the flat surfaces less expected.

Out of these considerations, a modification has been applied to rectangular and triangular particles. A small amount of face extension is applied to impacting surfaces of the particles to ensure an initial point contact. The change can be observed in Figure 2.51.

No-INF Model

Reasoning of the utilization of the half-infinite meshes is already done. The motivation is to avoid the reflection of dilatational and shear stress waves back into the model. However, this utilization creates some problematic issues as well.

Two sets of 100% coverage simulation files are combined to obtain one set of 200% coverage simulation file. It is noted that, in this type of high-coverage simulation files, model appears to show some errors after 150% coverage level. This error generally occurs at connection point of 3D stress elements and half-infinite elements.

To eliminate this error and make it possible to achieve high-coverage simulations, another type of model is considered. While keeping everything same in the same model, only the Substrate part is changed. In this new model, Substrate is modelled with no half-infinite elements but instead encastre boundary conditions at the side and bottom walls. Thus, model

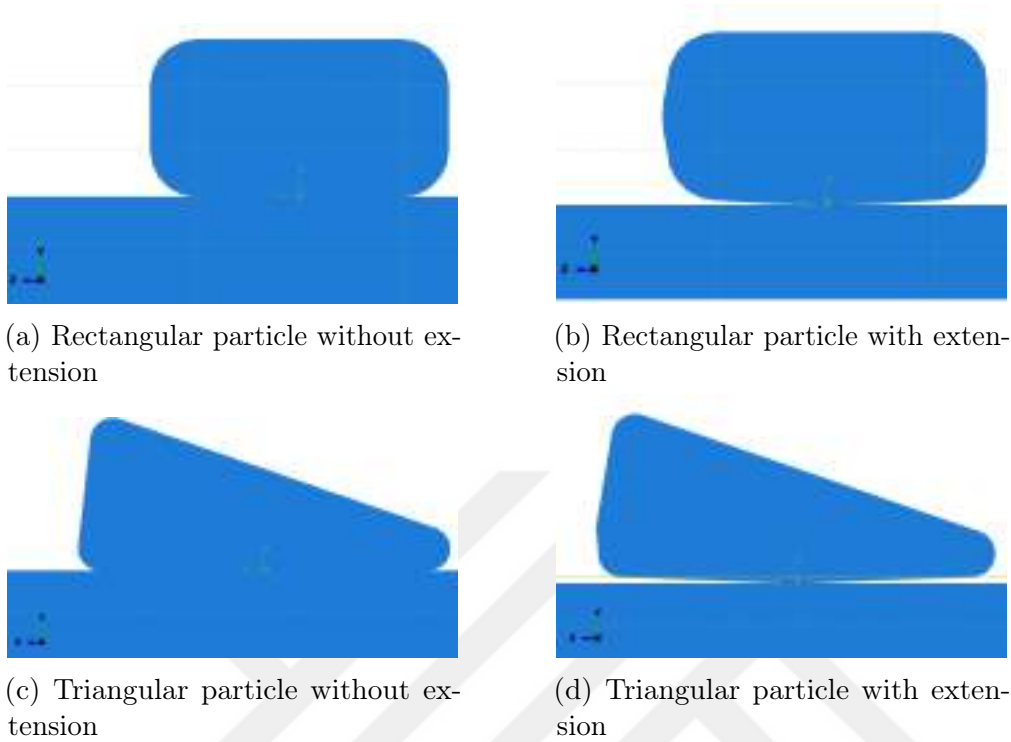


Figure 2.51: Modification visuals of rectangular and triangular particles

is fixed from all sides except impacted surface of the substrate. This new model is identified as “No-INF” model and its mainly utilized to see the results at different coverage levels. Other motivation is to see if there will be any error until 200% coverage level.

In Figure 2.52, the modification can be observed that is applied to the Substrate part.

While observing that extensions on rectangular and triangular particles are positively effecting the roughness parameters as they approach to the experimental results, model without half-infinite meshes is combined with extension particles to see the effect of extension also in that model as well.

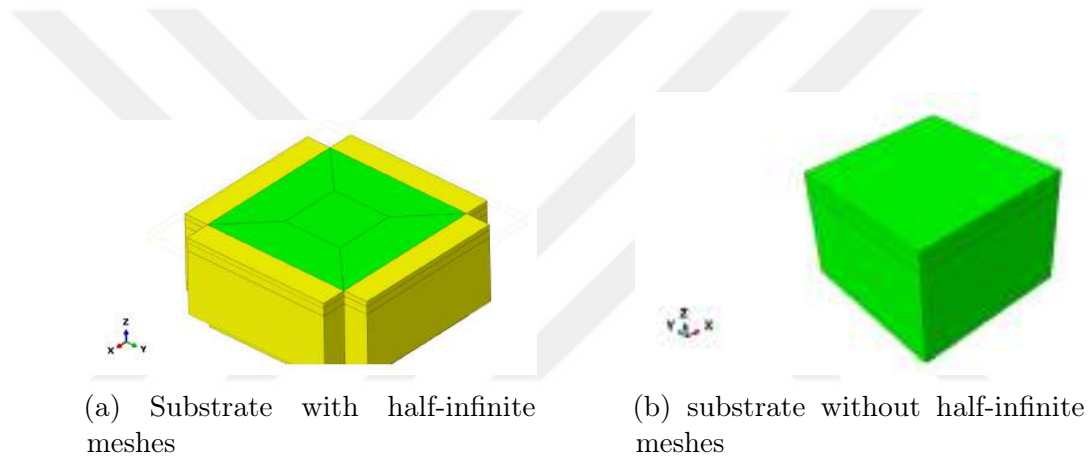


Figure 2.52: Visuals of substrate with half-infinite meshes and without half-infinite meshes

Chapter 3

Experimental Validation

3.1 Soft Blasting Equipment

Soft-blasting experiments in this thesis is done with machine, Guyson Formula F1600 that can be seen in Figure 3.1.



Figure 3.1: Guyson Formula F1600 machine

In general terms of the methodology, sand is accumulated in a box which has a connection with an external pipe that takes the sand through different set of phenomenons like suction or gravity depending on the equipment. As this sand-carrier pipe is connecting to the gun which also connects with air-supplier pipe, air and shot-media combine in the gun. Nozzle that is placed inside the gun is where air accelerates with its given pressure while also accelerating the shot particles. Air acts like the carrier of the particles and main accelerator. Given pressure of air and nozzle dimensions are the main contributions here for the air velocity. For the shot particle velocity, size, shape and density of the shots also become important contribution. Guyson Formula F1600 machine machine is shown in Figure 3.2



Figure 3.2: Guyson Formula F1600 machine

The nozzle utilized in Guyson Formula F1600 has an internal diameter of 8 mm and length of 65 mm. These dimension will play an important role in Step 2.3 of Chapter 2

The complete schematic with labelled parts of Guyson Formula F1600 can be seen in Figure 3.3 with names of each label in Table 3.1.

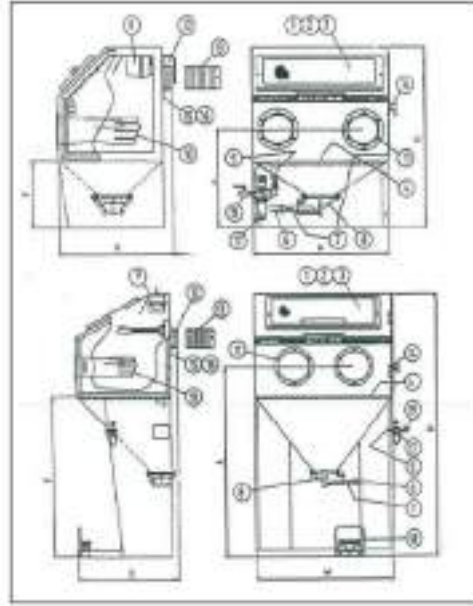


Figure 3.3: Guyson Formula F1600 machine schematic

3.2 Soft-Blasting Machine Stabilization

As mentioned in previous chapters, the 3 machine input parameters while conducting a soft-blasting operation on the machinery are:

- Air Pressure
- Stand-off Distance
- Impact Time (or Exposure Time)

N.Raghupathi [12] proposed same set of machine parameters for the experimental plan of his Master's thesis [12]. The purpose of that study was to examine the effect of these input machine parameters on different roughness parameters and eventually on wettability.

However, purpose of this study is to build a numerical model in order to simulate soft-blasting instead of analyzing the input effects separately. For this purpose, a relation must be constructed between machine parameters as the input of real-life operation and impact velocity as the input of numerical model with also contribution of the effect of material properties and dimensions of the nozzle utilized in the machine.

This relation is built and explained in Step 2.3 of Chapter 2. It can be seen in mentioned section that the only relative input machine parameters to impact velocity are Air Pressure and Stand-off Distance(SoD). Impact

Table 3.1: Component list of Guyson Formula F1600 machine

Number	Description
1	Viewing Window - 625 x 325 mm
2	Window Gasket
3	Antifrosting Sheet - 625 X 325 mm
4	Floor, Formula F1600
5	Air Hose, 10 mm bore
6	Media Hose - 16 mm bore
7	Pick-up Tube - 16 mm hose
8	Mixer Box
9	Bulkhead Light Fitting BC
10	Fixed Gauntlet - 26'
11	Armhole Bezel – Round - F1600
12	100 mm Dia Hose Spinning
13	Exhaust Hose 100 mm dia
14	Side Door Catch
15	Breather Pad
16	Breather Pad Bezel – Round
17	Combined Filter/Regulator
18	Foot Pedal Valve
19	Pneumatic Isolator 1/4" BSP

Time, as expected, has no effect on impact velocity.

While obtaining a specific set of input machine parameters for the experiments, impact time is required to be examined in the first place after some observations on the machine.

Before experiments are launched, several test trials are done on the ma-

chinery using experimental plan of N.Raghupathi [12] who separated the thesis into two as Preliminary Stage and Secondary Stage. In Preliminary Stage, the used values for the parameters are as the following:

- Air Pressure: 2-4-6 Bar
- SoD: 50-100-150 mm
- Exposure Time: 3-6-9 s

In this Preliminary Stage, PC is utilized as the substrate material. After the experiments of Preliminary Stage are completed, roughness measurements and consecutive studies are done and the observations required to reduce the parameter values to two as the following for Secondary Stage of the study:

- Air Pressure: 2-6 Bar
- SoD: 50-100 mm
- Exposure Time: 3-9 s

A new input parameter that is angle of impact is also input to Secondary Stage. The impacting angle is not covered in this study as the motivation is to build and validate a model that already has high amount of random factors.

It can be seen that, the limit values of Air Pressure and Exposure Time in Preliminary Stage are taken as inputs of Secondary Stage. On the other hand, 100 mm of SoD is chosen as an input in the Secondary Stage instead of 150 mm since it is observed that roughness parameters did not vary based on SoD going up to 150 mm from 100 mm.

The concept of this thesis requires to select a specific set of machine parameters and the launching point is Impact Time because initial tests performed on the machinery made the authors question the stability of the machine. The resulting surface morphology of the specimens were varying even with the same machine parameters. As the validation of the numerical model requires at least a reliable set of experimental results, there occurred a need to identify the best working condition of the machinery based on Impact Time parameter. For this purpose, a stabilization experiment is planned with the corresponding equipment as it can be seen in Figure 3.4.

The aim in this stabilization experiment is to run the machine and let it flow the shots out of the nozzle, not on a sample but into a box instead. Then by using a pressure balance, the mass of flowed shot particles are meant to be measured. The hypothesis was to observe a fluctuation in the mass of shot media with different trials of the same Impact Time.

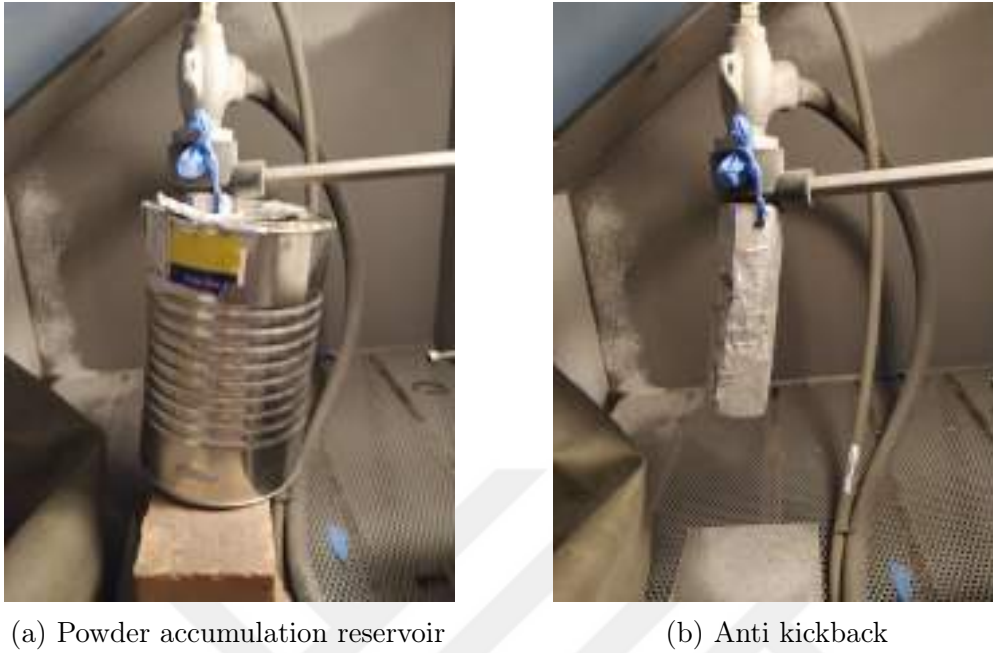


Figure 3.4: Volumetric flow rate equipment

Another observation from the initial tests was unstabilized performance of the machinery at low pressures like 2 Bar. As a result, consecutive steps are decided to be done in Pressure range of 4 Bar and 6 Bar with taking the note of best stabilized performances which are observed with 6 Bar.

Having processed this, an Impact Time Stabilization Experiment is planned both for pressure values of 4 Bar and 6 Bar. For each pressure it is planned to make the experiments for Impact Times of 1 s, 3 s, 5 s, 10 s and 60 s. For all Impact Time sets, tests are performed 5 times except 60 s test for which 8 tests are performed.

The mass of shot media that is obtained under all sets of Impact Times with 4 Bar of Air Pressure can be seen in Table 3.2 and the same set of values for 6 Bar of Air Pressure can be seen in Table 3.3.

The plots that are obtained from data of all time sets except 60 s can be seen in Figure 3.5 for 4 Bar and Figure 3.6 for 6 Bar.

The stabilization behavior is clearly observed from Table 3.2, Table 3.3 and correspondingly from Figure 3.5 and Figure 3.6. It is to be mentioned that the tests are done in down-to-up approach for the data in the tables. First step is to stabilize machine according to working pressure where machine runs for 60 s. Next step is to find at which time machine impacts the shot

Table 3.2: Impact Time Stabilization for 4 Bar

Time/Test	1	2	3	4	5
1	2.55	6.18	3.87	3.5	4.22
3	4.27	3.88	4.36	3.39	3.8
5	12.38	6.34	9.74	7.06	6.91
10	8.1	6.3	5.8	5.38	5.15

Table 3.3: Impact Time Stabilization for 6 Bar

Time/Test	1	2	3	4	5
1	21.22	28.47	13.11	16.31	6.53
3	32.74	17.19	21.01	23.22	15.05
5	30.26	16.84	32.4	21.84	15.99
10	13.71	26.16	20.62	42.4	33.05

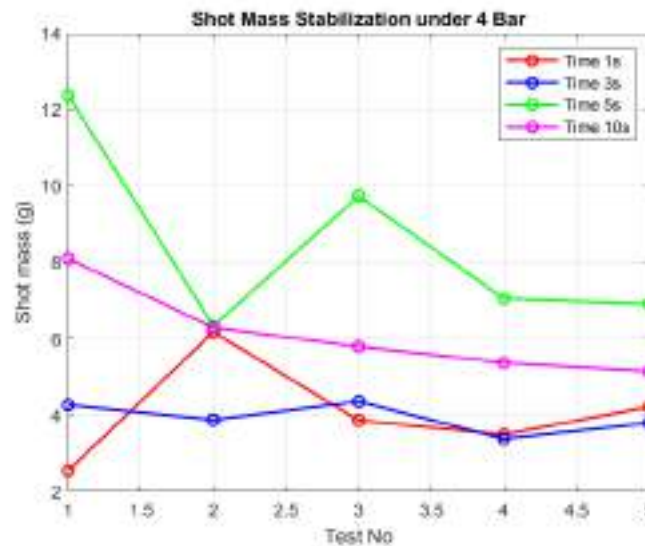


Figure 3.5: Impact Time Stabilization for 4 Bar

media on a stable level. It must be noted that, flow rate is also changing when pressure is changed. To stabilize flow rate machine needs to be

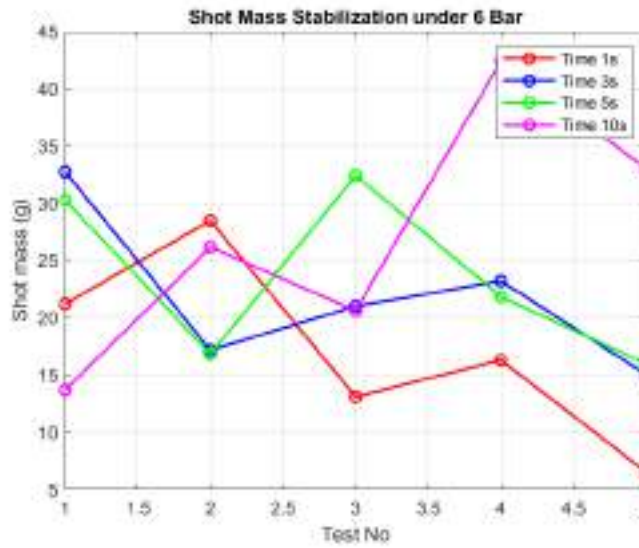


Figure 3.6: Impact Time Stabilization for 6 Bar

calibrated and this calibration procedure can be seen for 4 bar in Table 3.4 and for 6 bar in Table 3.5.

Table 3.4: Mass flow rate Stabilization for 4 Bar

Time/Test	1	2	3	4	5	6	7	8
60	530.1	205	191.3	139.2	146.7	99.7	133.7	117.6

Table 3.5: Mass flow rate Stabilization for 6 Bar

Time/Test	1	2	3	4	5	6	7	8
60	538.67	411.36	553.9	662.85	425.27	493.67	414.8	514.12

All of the first test of the impact sets have shown a high amount of shot collected in the box which clearly shows the effect of previous Impact Time. This is a clear indicator of machine unstability.

Concerning all the data obtained, it is decided to select 3 s of impact time in the main experimental procedure since shot mass variation was the least among all for 3 s both for 4 Bar and 6 Bar even if 3 s has also some variation.

This way, one of three main parameters (that we will be certified for the experiment set which will be utilized in the concept of validation) is selected.

The procedure requires the selection of the other two machine parameters selection which shall influence impact velocities of shot particles in the numerical model. The selection of the other two parameters is covered in the next chapter.

3.3 Experimental Plan

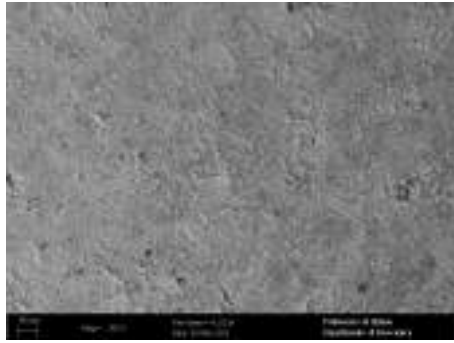
The selection of Air Pressure and SoD for the validation experiment set requires some decisive steps. As mentioned before, the machinery has also unstability based on the pressure. The surface morphologies obtained at different samples with 2 Bar of air pressure result differently even when it is visually checked.

Several preliminary tests showed that the best Air Pressure value to continue with is 6 Bar. Surface morphologies appear to not vary between different sets of samples with 6 Bar. Thus, the Air Pressure for Validation Experiment is selected as 6 Bar and the only remaining parameters to choose remained as SoD. To better visualize the effect of the pressure on coverage SEM images of gold coated impacted substrates are shown in Figure 3.7

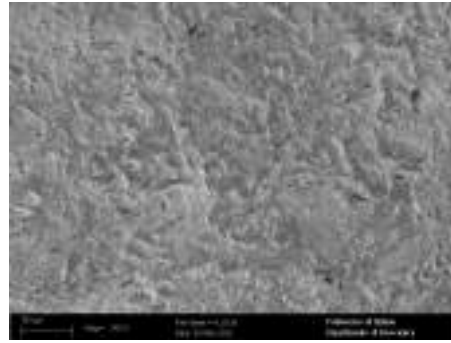
At this point, some sets of soft-blasting experiments are done with varying SoD between 100 mm, 150 mm and 200 mm while keeping the other parameters as 6 Bar for pressure and 3 s for impact time. The surface morphology of these samples are also examined for the selection of SoD for the validation set.

Before continuing with SoD selection, a different issue on the matter must be discussed which is Coverage Assessment on experimental samples. As explained with also citing the reference in the previous chapters, coverage is mainly the ratio of plastically deformed area to total area. Its determination by the users mainly rely on visual check.

However visual check requirement also brings a problem. This way it is not possible to detect coverage levels higher than 100%. Human eye can not detect how many times a point has been impacted. The only possible determination with visual check is the boundary of region that has 100% coverage. The user must detect the regions on samples where blank and unimpacted surfaces start to exist while going away from the impact center. These regions clearly mark the boundary point for 100% coverage. But it is a problematic issue to detect the coverage level of the regions between this boundary and the impact center.



(a) 6 bar, 100mm SoD, 3 seconds - magnification 200X



(b) 6 bar, 100mm SoD, 3 seconds - magnification 500X



(c) 4 bar, 100mm SoD, 3 seconds - magnification 200X



(d) 4 bar, 100mm SoD, 3 seconds - magnification 500X

Figure 3.7: SEM images of gold coated impacted surface under different pressures

Stereo microscopy can be utilized to process visual check on impacted samples. With different levels of magnification, one can detect the boundary for 100% coverage level. Stereo microscopy is also utilized in this thesis to examine soft-blasted samples. One representative figure can be seen in Figure 3.8.

Further analysis can also be done from images like Figure 3.8 to do automated checks and evaluate coverage. But as can be observed from Figure 3.8, soft-blasted surfaces tend to show a very irregular surface. This is mainly due to high irregularity of the shot media. This high irregularity creates very irregular surface characteristics making it a challenging task to examine the surface.

To better examine surface coverage assessment, SEM images of soft-blasted specimens were taken where substrate impacted surface coated with gold

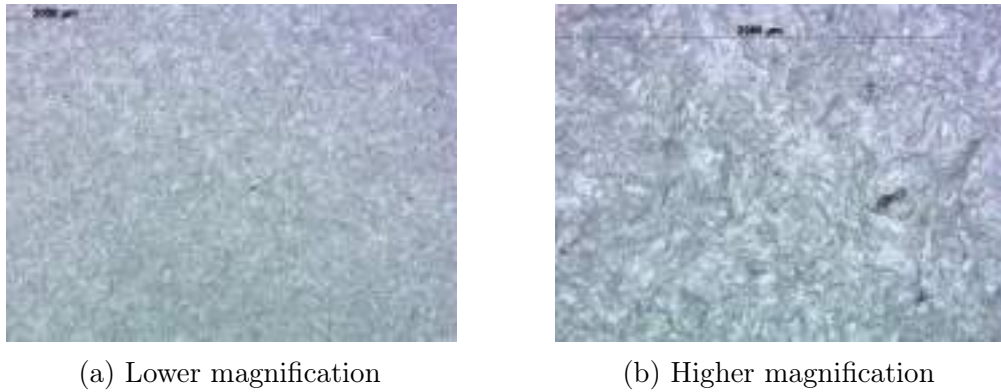


Figure 3.8: Stereo microscopy visuals of soft-blasted surface of PC under 6Bar and SoD of 150mm

to give conductivity. It can be observed that with machine parameters of 6Bar pressure and SoD of 150mm and impact time 3 second is reached 100% coverage. From the Figure 3.9 , with different variety of pressure, time and SoD effect can be examined.

One other issue is the chemical composition effect of shot media. As stated before, EDS analysis done on the shot media showed 90%-91% existence of Alumina in the powder and the remaining 9%-10% are belonging to different elements like Titanium (Ti).

During the high-velocity impacts Titanium leaves white color to impacted surface. This color is hard to clean off the surface by passing water only. It also requires hand contact which is not reasonable to operate on a sample which will then be taken to surface roughness measurement. To summarize, extra elements in the chemical composition of the powder leave unintended color intensity to sample surface as it can be seen in Figure 3.10. As image processing softwares work on color intensity, these unintended colors make it very difficult to operate.

The challenging task of coverage assessment on the experimental samples required a different perspective to the matter. The only descriptive information out of coverage assessment was the 100% coverage boundary. It is observed that on the samples of 6 Bar, 3 s and varying range of SoD (100 mm to 200 mm), 100% coverage boundary was around 10 mm radius distance from the impact center. A representative image taken around 10 mm distance from the impact center can be seen in Figure 3.11. In this figure, it is possible to observe unimpacted regions.



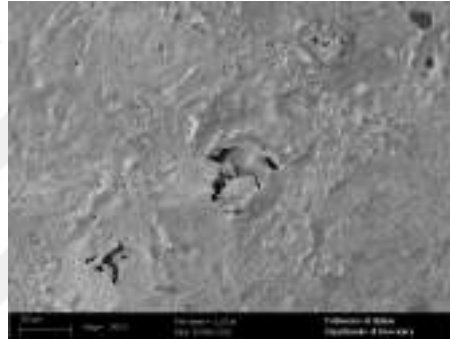
(a) 6 bar, 200mm SoD, 3 seconds - magnification 200X



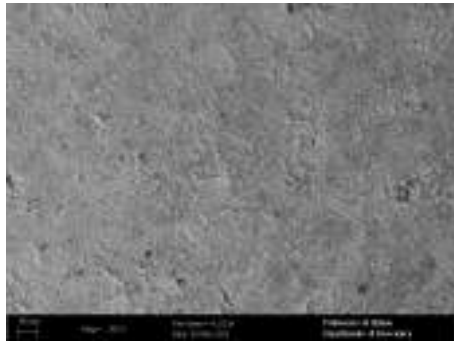
(b) 6 bar, 200mm SoD, 3 seconds - magnification 500X



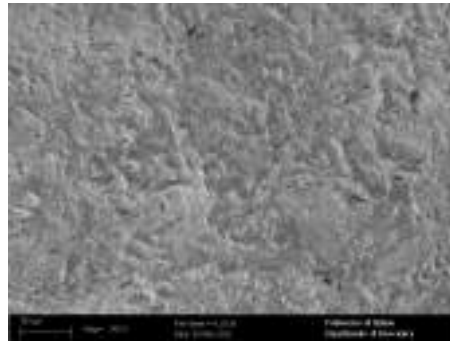
(c) 6 bar, 150mm SoD, 3 seconds - magnification 200X



(d) 6 bar, 150mm SoD, 3 seconds - magnification 500X



(e) 6 bar, 100mm SoD, 3 seconds - magnification 200X



(f) 6 bar, 100mm SoD, 3 seconds - magnification 500X

Figure 3.9: SEM images of gold coated impacted surface under different SoDs

The main problem here is the uncertainty of coverage level of impact center where impact velocities are already modelled in Step 2.3 of Chapter 2. On the other hand, coverage level on 100% coverage boundaries is known but

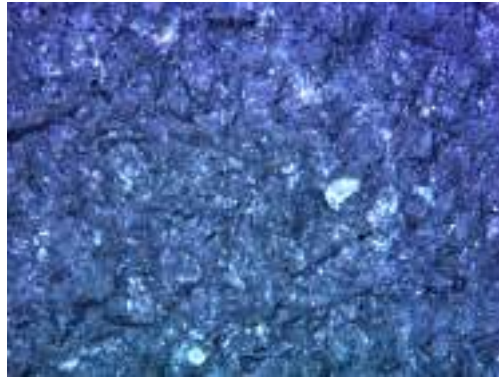


Figure 3.10: White mark on visual of Stereo microscopy

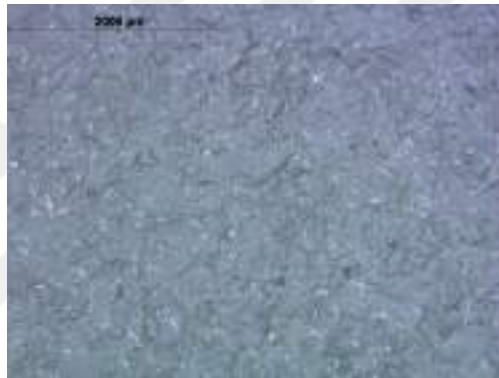


Figure 3.11: Representative visual of not impacted regions

this time impact velocity in this region is unknown as the particle velocity model mainly predicts the particle velocity in the impact center.

Having observed this, a further examination on the samples brought the selection of 150 mm for SoD, since particle velocity model predicts that the velocity will be more or less equal between SoD range from 100 mm to 250 mm and a very small velocity lowering for 50 mm of SoD. In fact, coverage visual check showed that the most observable coverage boundary level was obtained with 150 mm of SoD. For higher SoD values, particle velocities are expected to be same but the jet expansion through particle travel made the jet stream impact on a wider area and thus effecting the coverage levels. Having more clear and more observable boundary coverage levels ensured the selection of 150 mm for SoD.

Having clarified the last parameter, validation experiment set is complete and can be observed in Table 3.6.

Table 3.6: Experimental validation parameters

Air Pressure[Bar]	SoD[mm]	Impact Time[s]
6	150	3

3.4 Measurement

Three different samples of PC are soft-blasted in total with the machine parameters that are clarified at previous chapter. The experiment is done more than once in order to increase the experimental data set and thus the accuracy of the results.

A measurement methodology is also considered. As mentioned before, ISO-4288 is being applied for measurement of roughness both in numerical and experimental model.

The selection of 0.25 mm of cut-off wavelength between different cut-off standards of ISO-4288 was already explained. Here again, cut-off wavelength is selected as 0.25 mm which requires a total evaluation length of 1.25 mm.

The measurement methodology is an outcome of limited coverage assessment done in the previous chapter. As it is explained, 100% coverage zone covers a zone with around 10 mm radius as visually observed. The measurements must therefore provide the information of roughness in a zone that is smaller than 10 mm radius circle.

For this purpose, it is planned to make 7 measurements on each sample and thus obtaining 21 measurements from all 3 samples in total. The measurements will be done on Mahr PGK Perthometer. Figure 3.12 shows a representative image from Measurement phase of the study.

ISO-4288 provides the information that the measurements that are done with 0.25 mm of cut-off wavelength should also be done with a probe tip that has a radius of 2 μm . This probe tip radius acts like a filter over measurement and it is used as the standard.

Probe will move on single-direction path for a distance of measurement length (=1.75 mm) in which it will do the surface measurement for a distance of evaluation length (=1.25 mm) and it will sample the data into 5 each having a distance of sampling length (=cut-off wavelength=0.25 mm). Eventually, following roughness parameters will be evaluated:

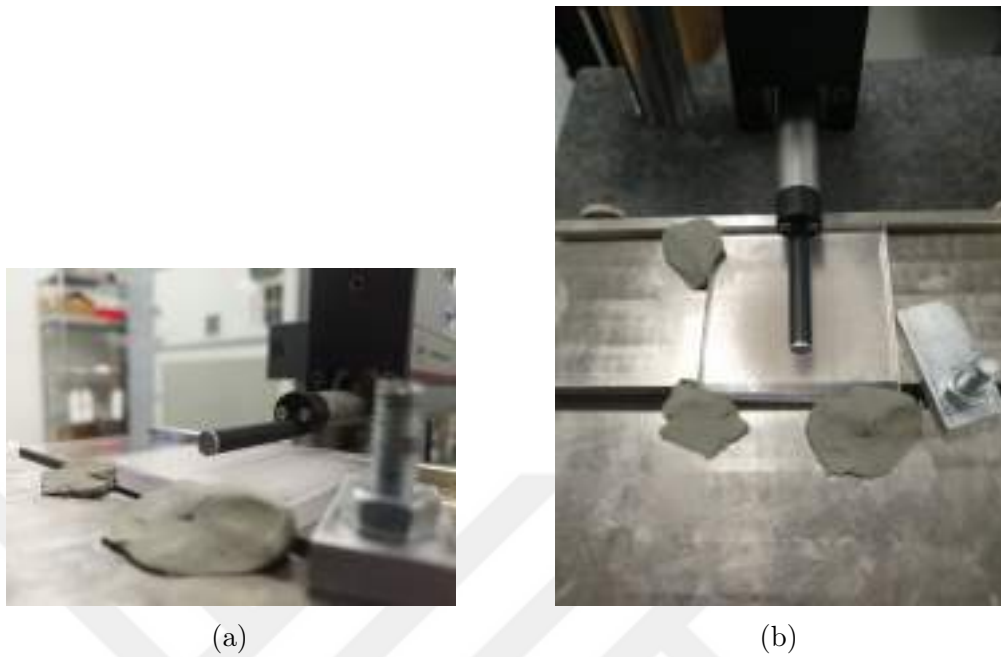


Figure 3.12: Experimental measurement set up on Mahr PGK Perthometer

- R_a
- R_q
- R_z
- R_t
- R_{max}

As these parameters are also outputs of complete numerical model, validation of the model will take place upon them.

As probe will move and measure along 1.25 mm distance, it is decided to make the multiple one-direction measurements leaving a space of 1.25 mm within the closest measurement lines. That represents the main reasoning behind having 7 measurements on one sample. As there will be 1.25 mm of distance between measurements, they will cover a range of -3.75 mm to 3.75 mm of distance to impact center.

The image for measurement procedure can be seen in Figure 3.13.

Obtaining roughness values at a distance of 3.75 mm from the impact center collaborates with the idea of getting the roughness inside 10 mm radius circle which seems to have at least 100% coverage.

Combining the measurement procedure with the limited coverage assess-

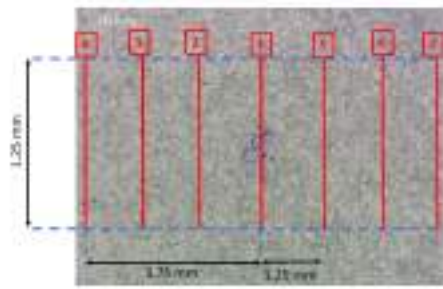


Figure 3.13: Experimental roughness measurement procedure

ment, the following validation procedure for the model is decided and utilized.

- As it is not possible to know the exact coverage level of the impact zone, all the roughness values measured in the center distance range of -3.75 mm to 3.75 mm will be taken into consideration. If their values do not show a great variability, the mean of these values will be used to compare with the numerical data
- Numerical model will be run for multiple times and for each model set, results will be compared with the average values of roughness parameters for all 21 experimental measurements. All experimental results can be examined in Appendix A.1

A further concept must be explained here, as the results will be obtained with a cut-off wavelength of 0.25 mm, this value should be indicated at all the steps of the process. Even the future studies concerning wettability should have the indication of it since cut-off wavelength is the most important filtering step in the post processing operation of both the numerical model and experimental model. Changing this value would also change the results. To limit the misunderstandings about the final surface roughness parameters, indicating the cut-off wavelength is at utmost importance.

Chapter 4

Results and Discussion

As already explained, a specific set of machine parameters is utilized to process in the experiments. The roughness parameters obtained from the impact center zone of these samples will represent a validation data upon which the difference percentage will be calculated for each parameter.

In the last section of Chapter 2, two further enhancement to the built model are introduced. The results here will be presented in a way to demonstrate the effect of these modifications. The results obtained with the built model will firstly be shown and then followed by the results of models with enhancements.

The built model and extension enhancement (to ensure initial point contact instead of face contact during impacting of rectangular and triangular shot particles) will be shown over 6 simulation sets of which each has 100% coverage level. On the other hand, No-INF model and the extension enhancement on it will be shown over 3 simulation sets of which each has 200% coverage level.

Cut-off wavelength is applied as 0.25 mm in both numerical and experimental processes. For this cut-off wavelength, ISO-4288 requires to use 2 μm radius for the probe tip. The validation tools will be the mean comparison bar plot with standard deviations plotted on and the roughness parameters development plot based on the measurement number. In the latter plot, numerical results that are obtained in two directions as much as the smoothing points number for each direction (1000 is utilized in the model), will be segmented into pieces as much as the total measurements number which is 21 (7 measurements on each sample and 21 measurements on total 3 samples). A supplementary table will also be provided showing

the mean roughness parameters of numerical and experimental processes with also their difference percentage.

For the sake of simplicity, roughness development plots will only be shown for Simulation Set-1 of built model which consists of half-infinite elements. For the rest, the comparison and validation tools will be as the following:

- Bar Plot of Experimental and Numerical Results without Extension Enhancement
- Bar Plot of Experimental and Numerical Results with Extension Enhancement
- Summary Table including mean results of models with difference percentage

Numerical simulation with No-INF model, goes up to 200% coverage as this was one of the motivations of processing this model. So these results will be shown after 100% coverage and after 200% coverage. The percentage difference with the experimental results will be given over the results of 200% coverage.

Results of Model with Half-Infinite Meshes

Simulation Set-1

The results of Simulation Set-1 with comparison to Experimental Results are shown in Figure 4.1 without extension effect and Figure 4.2 with extension effect.

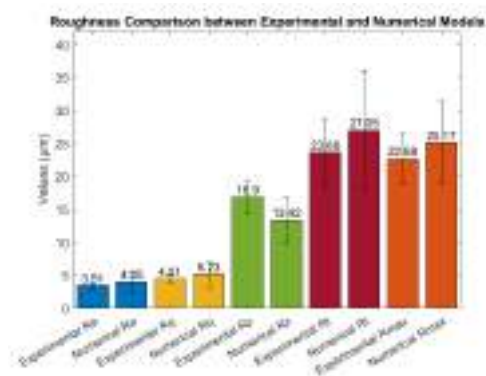


Figure 4.1: Set-1 bar plot without extension

Extension effect appears to reduce difference percentage especially in Ra parameter value.

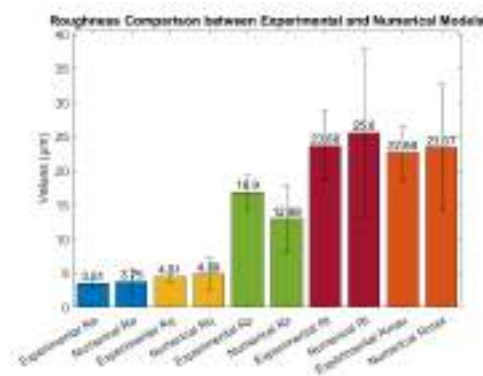


Figure 4.2: Set-1 bar plot with extension

In both cases the results demonstrate a good matching with the experimental results. Considering the fact that, this model is built as a novel way to simulate soft-blasting and has particular differences than shot peening and its simulation, 30% of difference was considered to be hypothetically satisfying. All of the roughness parameters are below this percentage as they can be seen from Table 4.1. Even for Ra and Rq which are the parameters that define the roughness state on a more global scale, the difference is under 20%.

Table 4.1: Set-1 all results

	Ra	Rq	Rz	Rt	Rmax
Experimental Results	3.51	4.51	16.90	23.68	22.68
Without-Extension-Numerical Results	4.05	5.23	13.42	27.05	25.17
Without-Extension-Difference (%)	15.18	16.16	20.60	14.24	10.97
With-Extension-Numerical Results	3.75	4.89	12.99	25.60	23.37
With-Extension-Difference (%)	6.84	8.60	23.10	8.08	3.04

Set-1 results clearly show the positive effect of extension on rectangular and triangular part faces. The model with extension demonstrates an enhancement with difference around 6% for Ra, 8% for Rq and Rt and even 3% for Rmax and 23% difference for Rz which is still under acceptable threshold. It must be noted that, out of these parameters Rmax is the one that has the probability to show the local effect. Achieving low difference on this value shows that the random impact particle sequence of this set is matching quite well with the reality.

As specified before, solely for Set-1, roughness development plots through measurements of all 3 samples will be shown. The model successfully plots

and saves these for all simulation sets. In order not to lead a crowded data on the thesis, they will be only shown for Set-1.

These plots can be seen in Figure 4.3.



(a) Experimental Ra value comparison with numerical simulation



(b) Experimental Rq value comparison with numerical simulation



(c) Experimental Rz value comparison with numerical simulation



(d) Experimental Rt value comparison with numerical simulation



(e) Experimental Rmax value comparison with numerical simulation

Figure 4.3: Reference model

Simulation Set-2

The results of Simulation Set-2 with and without extension effect can be examined from Figure 4.4, Figure 4.5 and Table 4.2.

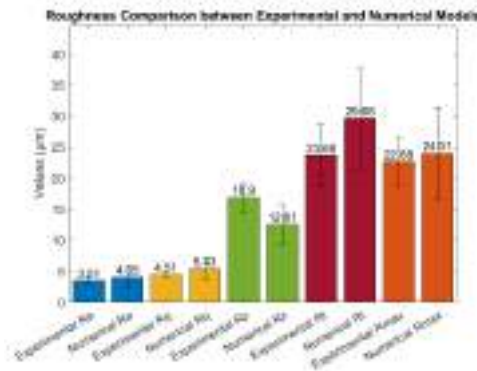


Figure 4.4: Set-2 bar plot without extension

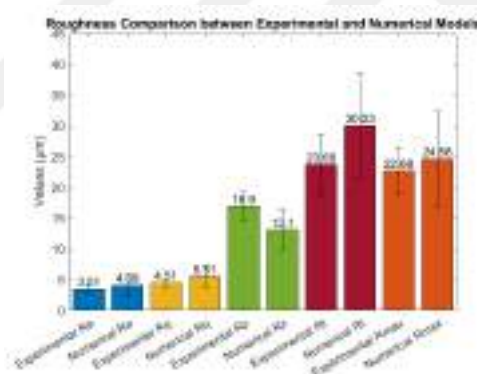


Figure 4.5: Set-2 bar plot with extension

Table 4.2: Set-2 all results

	Ra	Rq	Rz	Rt	Rmax
Experimental Results	3.51	4.51	16.90	23.68	22.68
Without-Extension-Numerical Results	4.05	5.43	12.61	29.66	24.01
Without-Extension-Difference (%)	15.16	20.60	25.37	25.23	5.86
With-Extension-Numerical Results	4.08	5.51	13.10	30.03	24.58
With-Extension-Difference (%)	16.25	22.20	22.50	26.78	8.35

In the result of Set-2, extension effect does not reduce percentage difference in roughness parameters except Rz. In the other parameters, the change is

almost negligible yet the percentage difference with extension effect still remains under acceptable threshold.

Simulation Set-3

The results are summarized in Figure 4.6, Figure 4.7 and Table 4.3.

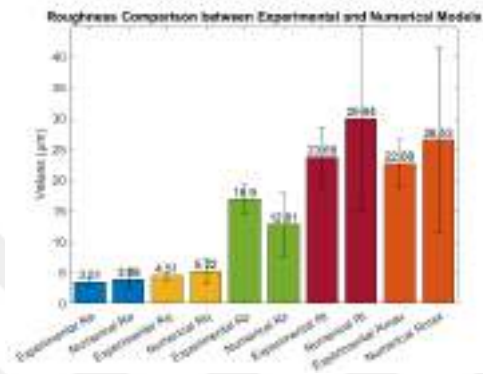


Figure 4.6: Set-3 bar plot without extension

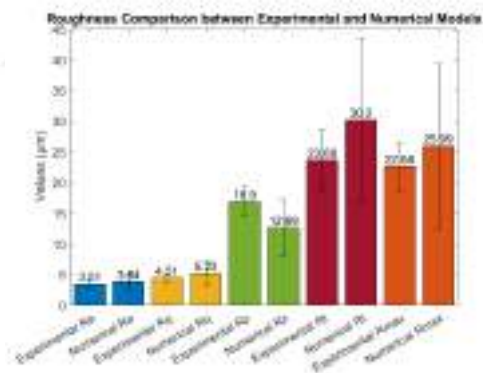


Figure 4.7: Set-3 bar plot with extension

Table 4.3: Set-3 all results

	Ra	Rq	Rz	Rt	Rmax
Experimental Results	3.51	4.51	16.90	23.68	22.68
Without-Extension-Numerical Results	3.88	5.22	12.81	29.94	26.53
Without-Extension-Difference (%)	10.48	15.92	24.17	26.44	16.95
With-Extension-Numerical Results	3.84	5.23	12.69	30.20	25.99
With-Extension-Difference (%)	9.45	16.12	24.91	27.52	14.59

Table 4.3 shows that the results of Simulation Set-3 shows better percentage difference especially for Ra parameter. Extension effect still does not have big impact though but compared to Simulation Set-2, small change in Ra occurred to have a positive effect this time.

Simulation Set-4

The following results shown in Figure 4.8, Figure 4.9 and Table 4.4 are obtained for Simulation Set-4.

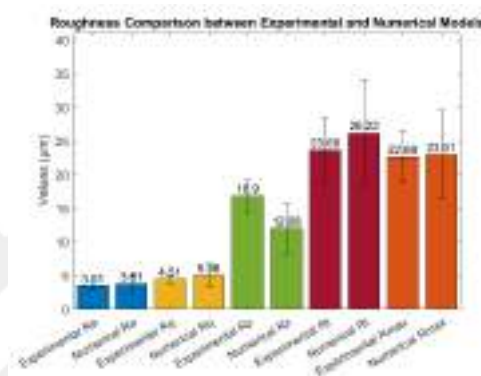


Figure 4.8: Set-4 bar plot without extension

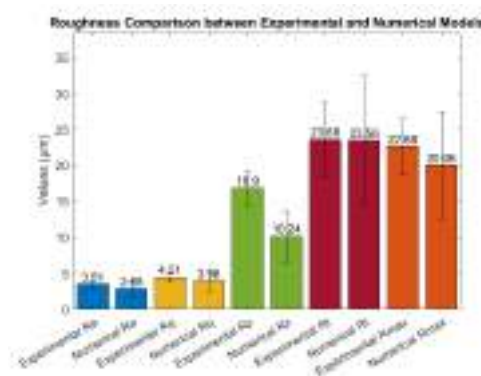


Figure 4.9: Set-4 bar plot with extension

Set-4 achieves the best ever results in the case of no extension applied. Having 8% percentage in Ra parameter clearly shows a very close value to experimental results. On the other hand, extension has a negative effect here which needs a deep consideration. For this, Figure 4.10 can be examined.

Table 4.4: Set-4 all results

	Ra	Rq	Rz	Rt	Rmax
Experimental Results	3.51	4.51	16.90	23.68	22.68
Without-Extension-Numerical Results	3.81	5.08	12.08	26.22	23.01
Without-Extension-Difference (%)	8.36	12.73	28.50	10.70	1.42
With-Extension-Numerical Results	2.88	3.98	10.24	23.56	20.06
With-Extension-Difference (%)	18.04	11.62	39.40	0.54	11.54

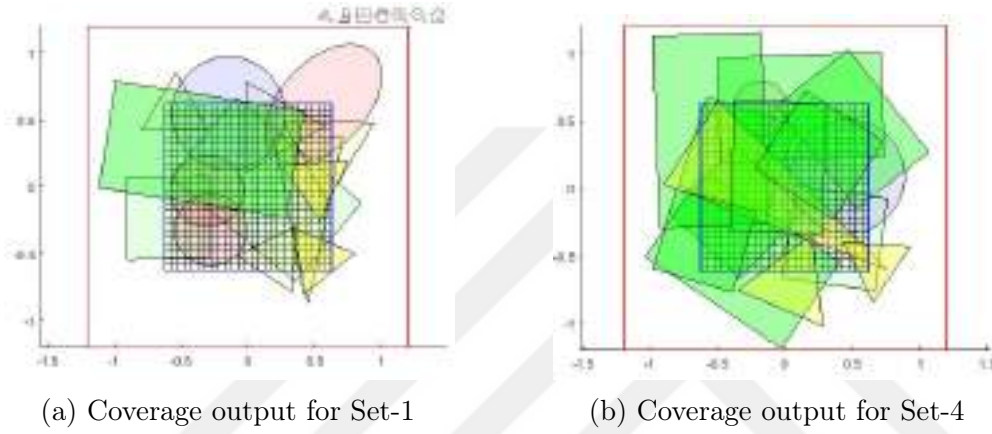


Figure 4.10: Matlab coverage output visuals

Figure 4.10 shows the random particle distribution for Set-1 and Set-4 on the impact zone consecutively. It is clearly seen that, Set-1 has a better dispersed particle distribution and the number of groups and sub-groups of the shot particles appear to have a homogeneous dispersion. However for Set-4, the random impact sequence mainly input the rectangle particle impacts on the zone.

Two main explanations can be done here:

1. Set-4, which is mostly rectangular particles gives the least percentage difference.
2. Extension that is applied to rectangular and triangular particle surfaces has a negative effect when the impact sequence has a tendency for rectangular and triangular particles.

The reasonings and possible further indications will be covered in Conclusion chapter.

Simulation Set-5

The results of Set-5 are given in Figure 4.11, Figure 4.12 and Table 4.5

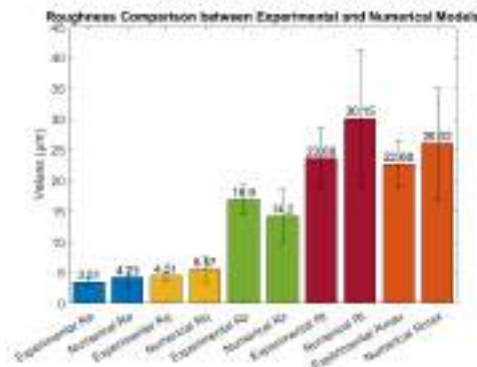


Figure 4.11: Set-5 bar plot without extension

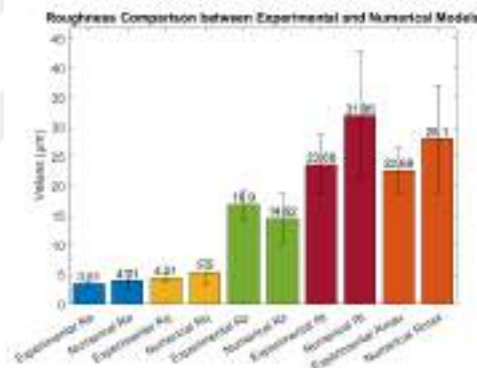


Figure 4.12: Set-5 bar plot with extension

Table 4.5: Set-5 all results

	Ra	Rq	Rz	Rt	Rmax
Experimental Results	3.51	4.51	16.90	23.68	22.68
Without-Extension-Numerical Results	4.23	5.57	14.20	30.15	26.02
Without-Extension-Difference (%)	20.48	23.70	15.96	27.30	14.72
With-Extension-Numerical Results	4.01	5.50	14.62	31.96	28.10
With-Extension-Difference (%)	14.09	22.05	13.46	34.94	23.86

It can be seen from Table 4.5 that percentage difference of Ra, Rq and Rz decreased with the utilization of the extension. However, percentage difference for Rt and Rmax increased. This is due to the local effect that

the extensions are causing. The results of Set-5 contributes to the accuracy of the model as the results are inside the accepted thresholds. Once again extension appears to have a positive effect on the results.

Simulation Set-6

Figure 4.13, Figure 4.14 and Table 4.6 shows the results of Simulation Set-6.

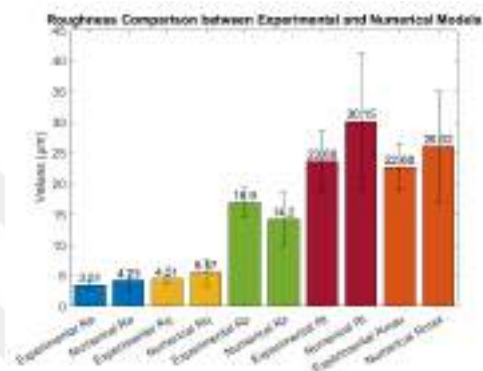


Figure 4.13: Set-6 bar plot without extension

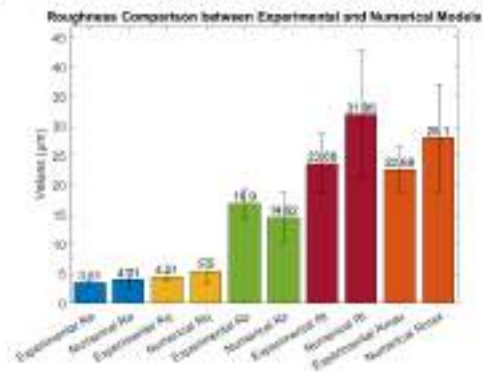


Figure 4.14: Set-6 bar plot with extension

Just like Simulation Set-5, here again extension has a positive effect on Ra, Rq and Rz. On the other hand, the effect tends to increase percentage difference for Rt and Rmax.

Having most of the parameters in the acceptable level, Set-6 also validates the numerical model. Extension has a depending effect on the parameters but the positive effect is obvious in Ra parameter.

Table 4.6: Set-6 all results

	Ra	Rq	Rz	Rt	Rmax
Experimental Results	3.51	4.51	16.90	23.68	22.68
Without-Extension-Numerical Results	4.13	5.47	14.02	31.99	26.98
Without-Extension-Difference (%)	17.48	21.48	17.01	35.06	18.94
With-Extension-Numerical Results	3.84	5.42	14.37	34.25	29.48
With-Extension-Difference (%)	9.25	20.21	14.95	44.64	29.98

Results of Model without Half-Infinite Meshes

As specified before, the reasoning behind utilization of model without half-infinite meshes is to avoid the errors that occur after 150% coverage level in consecutive impact sequences as these errors tend to be formed at connection point of 3D stress and half-infinite elements.

There are 3 simulation models in this set of Results each has been run for 200% coverage simulation which means two sets of consecutive simulations that are individually gathered for 100% coverage on each. To show the behavior of the model, results that are obtained after both 100% coverage and 200% coverage will be shown.

One other aspect here is that, the impact square is input as 2.5 mm in this case rather than 1.25 mm. Thus, the results that will be shown will be the roughness parameters resulting from the surface morphology of a soft-blasted 2.5 mm x 2.5 mm surface.

The required comprehensions will be done after demonstrating the results.

Simulation Set-N1

Figure 4.15 and Table 4.7 shows the results of Simulation Set-N1. Figure 4.15 is a combination of 4 bar plots where the roughness parameters are plotted with comparison to experimental results after 100% and 200% coverage both before extension and after extension. Same presentation procedure will also be applied for Simulation Set-N2 and Simulation Set-N3.

A summary table is also provided as Table 4.7 where the mean values are also combined with percentage differences which may contribute to the comprehension of effects done by enhancements made on the model.

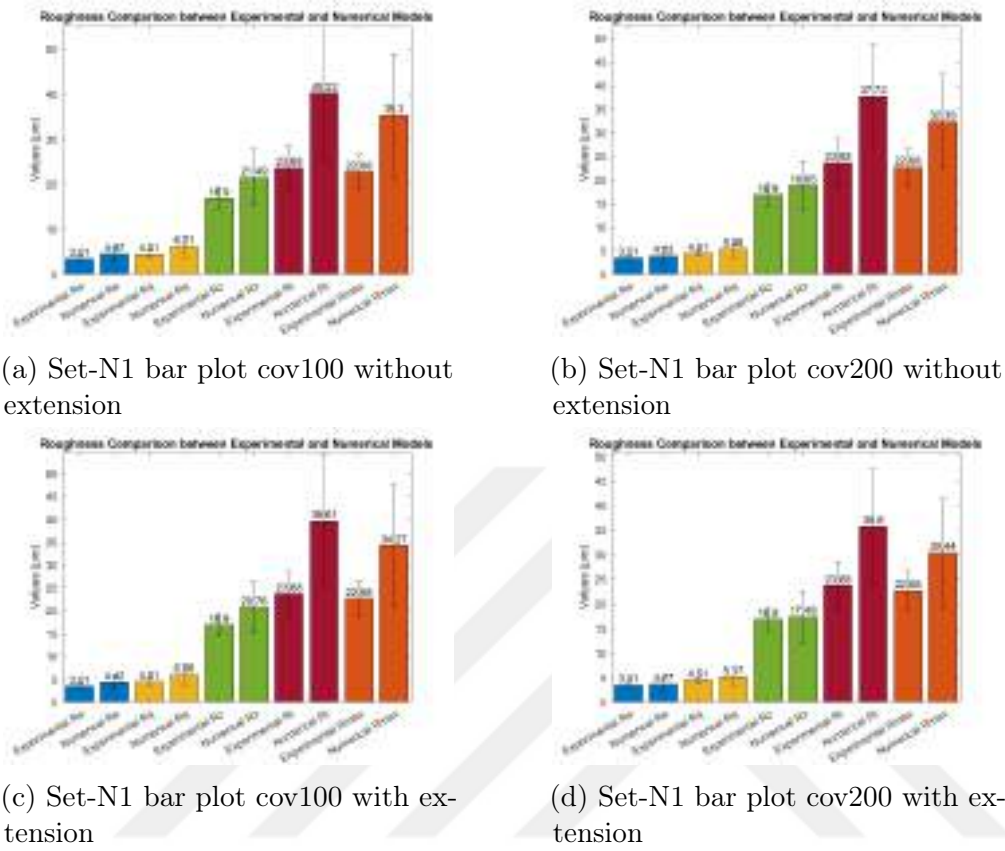


Figure 4.15: Set-N1 all bar plots

Table 4.7: Set-N1 all results

	Ra	Rq	Rz	Rt	Rmax
Experimental Results	3.51	4.51	16.90	23.68	22.68
Without-Extension-Cov100-Numerical Results	4.57	6.21	21.49	40.22	35.30
Without-Extension-Cov100-Difference (%)	30.20	37.84	27.20	69.83	55.61
With-Extension-Cov100-Numerical Results	4.42	6.08	20.76	39.61	34.27
With-Extension-Cov100-Difference (%)	25.71	34.82	22.88	67.25	51.10
Without-Extension-Cov200-Numerical Results	4.02	5.48	18.85	37.72	32.39
Without-Extension-Cov200-Difference (%)	14.46	21.67	11.57	59.28	42.78
With-Extension-Cov200-Numerical Results	3.77	5.17	17.49	35.80	30.44
With-Extension-Cov200-Difference (%)	7.34	14.64	3.53	51.18	34.22

Simulation Set-N2

Figure 4.15 and Table 4.8 summarizes the results obtained for Simulation Set-N2.

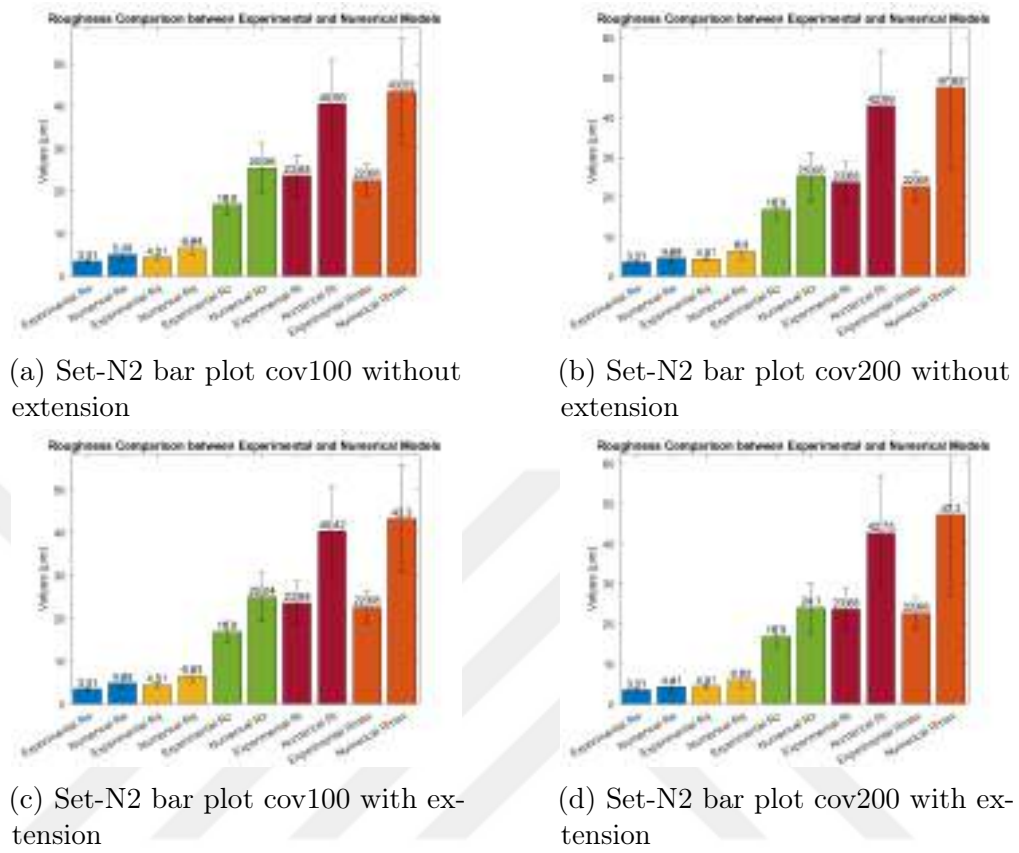


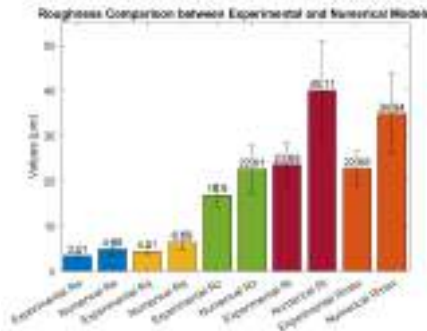
Figure 4.16: Set-N2 all bar plots

Table 4.8: Set-N2 all results

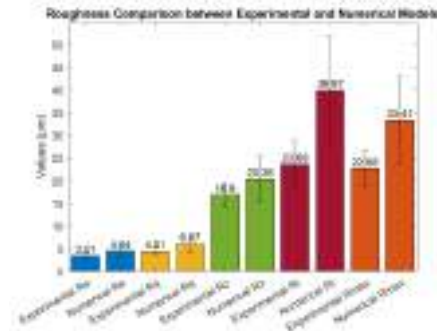
	Ra	Rq	Rz	Rt	Rmax
Experimental Results	3.51	4.51	16.90	23.68	22.68
Without-Extension-Cov100-Numerical Results	5.18	6.84	25.56	40.56	43.52
Without-Extension-Cov100-Difference (%)	47.47	51.69	51.24	71.28	91.87
With-Extension-Cov100-Numerical Results	4.95	6.63	25.04	40.42	43.30
With-Extension-Cov100-Difference (%)	40.82	47.22	48.16	70.65	90.90
Without-Extension-Cov200-Numerical Results	4.69	6.30	25.08	42.99	47.69
Without-Extension-Cov200-Difference (%)	33.55	39.88	48.44	81.51	110.26
With-Extension-Cov200-Numerical Results	4.41	6.02	24.10	42.75	47.30
With-Extension-Cov200-Difference (%)	25.66	33.60	42.60	80.51	108.54

Simulation Set-N3

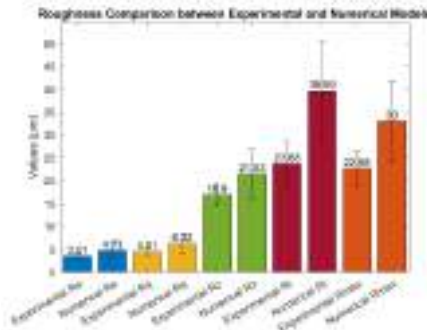
Figure 4.17 and Table 4.9 are provided to summarize the results of Simulation Set-N3.



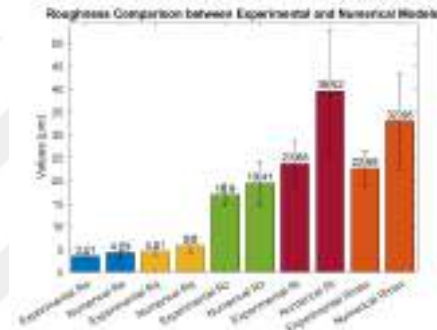
(a) Set-N3 bar plot cov100 without extension



(b) Set-N3 bar plot cov200 without extension



(c) Set-N3 bar plot cov100 with extension



(d) Set-N3 bar plot cov200 with extension

Figure 4.17: Set-N3 all bar plots

Table 4.9: Set-N3 all results

	Ra	Rq	Rz	Rt	Rmax
Experimental Results	3.51	4.51	16.90	23.68	22.68
Without-Extension-Cov100-Numerical Results	4.98	6.59	22.61	40.11	34.94
Without-Extension-Cov100-Difference (%)	41.71	46.35	33.78	69.36	54.03
With-Extension-Cov100-Numerical Results	4.73	6.32	21.53	39.59	33.00
With-Extension-Cov100-Difference (%)	34.53	40.29	27.39	67.18	45.49
Without-Extension-Cov200-Numerical Results	4.54	6.07	20.38	39.97	33.41
Without-Extension-Cov200-Difference (%)	29.13	34.65	20.63	68.77	47.27
With-Extension-Cov200-Numerical Results	4.29	5.80	19.41	39.52	32.98
With-Extension-Cov200-Difference (%)	22.06	28.78	14.89	66.87	45.41

As all the results are plotted with the corresponding tables, some general comprehensions can be drawn.

Inside the set of roughness parameters that are used to validate the data, Ra and Rq is the most global ones as they are respectively average of

absolute values and root mean square of the roughness data. The other parameters can be easily influenced by some local effects, this makes Ra and Rq most characterizing parameters of the surface.

Having said this, it must be also stated that the other parameters shall also be close to acceptable level of difference percentage since shot particle characterization that is done in Step 2.2 of Chapter 2 develops the particle geometries and tries to gather the 3D dimensions. The results show that even these possibly local-influencing parameters have higher percentage differences they seem to be inside or around acceptable level of difference.

The originally built model with half-infinite meshes and without extensions has good matching with the experimental results. Among 6 observations, Ra value has the lowest difference of 8% and highest difference of 20%. The most characteristic property of surface roughness has considerably acceptable results with regards to 30% threshold for percentage difference.

Among the examined literature, Bagherifard et al. [16] demonstrated a good matching between experimental and numerical findings. The highest difference is around 11%. Mylonas et al. [22], showed a not very well matching between numerical and experimental results especially with increasing the shot velocity. Ghasemi et al. [28] evaluated 2.6% difference but on the coverage level of 1000%. The results demonstrated by Bhuvvaraghan et al. [21] shows a 17% difference and the resulting plots of Wu, Liu and Wei et al. [30] show to have a 33% difference between experimental and numerical findings. Considering these results from the literature, providing a difference around 8% as the minimum and 20% as the maximum puts the study in a good position among the literature.

The model that is enhanced with extensions and still utilized within half-infinite meshes has a dependable effect on the results. If the impacting sequence is composed of a well-mixed fraction of particle groups, extension either has negligible effect or positive effect. On the other hand, if the impacting sequence has a dominance of flat-contact particles (i.e. rectangular and triangular particles), the results seem to go worse. The results of Simulation Set-1 show that after extension, Ra difference goes down to 6% which is a better result than the best of the results obtained for the simulations of models without extension that is around 8%.

It can be noted that, the best results in the model without extension enhancement is obtained with the model which is the only model that has worse results after extension. The peculiarity of this model is the dominance of rectangular parts. It can be stated that, the particles in the

shot media have a tendency over rectangular particles. In other words, these results show that particle characterization can be even improved with considering a high number of rectangular particles instead of spherical or ellipsoidal particles.

The model that has the replacement of Encastre boundary conditions instead of half-infinite meshes appear to have a high variety of result quality. First issue to mention is that the hypothesis of no-error simulation is achieved and in this way, simulation goes up to 200% coverage without errors that have a tendency to pop-up in the model with half-infinite meshes after 150% coverage level.

On the contrary, results seem to have got worsened. The reason of half-infinite mesh utilization in the model is to avoid the reflection of stress waves that translate through side walls after impact. The results of these model shows that, this reflection phenomenon clearly effects the results. Thus, it is not reasonable to utilize this model and it is obviously better to continue the model with half-infinite meshes even if elimination of half-infinite meshes also eliminated possible error causes.

As the model without half-infinite elements go over 100% coverage to 200% coverage, the effect of coverage can be evaluated on surface roughness final results. As Table 4.7, Table 4.8 and Table 4.9 show, most of the roughness parameters are decreased while coverage goes up. This is indicating that, surface state tends to have a more flat-like shape as the consecutive impact sequences progress.

One last point to cover in the model without half-infinite meshes is the positive effect of extension. Even if no-infinite model results do not have a good matching, extension clearly enhanced the results. It is considered that keeping the extensions in the model is reasonable and the consecutive studies must be done including the extensions.

Through all simulation and experimental findings, it can be said that the difference between numerical and experimental findings can be attributed to two causes:

- 1) Manual influence on shot particle characterization: The simulation with dominant number of rectangular shot particles gives the best result. This shows the tendency of the shot media to be characterized more like rectangular particles.

2) Variation of material properties: The meshes in the impact zone of FEA model will deform based on material properties input. As the concept of thesis also includes a validation phase for the model with the experimental findings, one must be sure that material properties reflect the real time case. However, material properties tend to vary even between same set of material while only varying the manufacturer. In other words, gathering a common material information into FEA model may over/underestimate final results.

Finally, as it is considered to continue with the model that is equipped with extensions on rectangular and triangular particle surfaces as well as half-infinite meshes at the side walls of Substrate instance, the results of these model should be mentioned. This model achieved the best result of difference of 6% based on Ra, which shows a great matching with the experimental results. The worst matching is 18% based on Ra results which, as shown before, is quite rare impact sequence to expect but still demonstrating an acceptable level of percentage difference.

Chapter 5

Conclusion

The motivation of this Thesis is to build a numerical model that acts like an interface to simulate soft-blasting process which seems promising since it would decrease the experimental effort that needs to be put into the studies.

The objectives of the Thesis are :

- 1) Construct a model that take soft-blasting machine parameters and material properties as input and give surface roughness values as outputs.
- 2) Provide a model that is ready to be contributed by wettability examinations for the future studies.

In the concept of this thesis, a numerical model is built which takes into account several parameters of the process like the material properties of the impacting shot media and polymeric substrates, geometrical dimensions of irregular shot media, machine parameters like pressure and stand-off distance. The model is also equipped with several scripts that would work in collaboration to characterize shot media, evaluate shot impact velocity, induce several randomness factors and arrange the post-processing steps to gather roughness parameters. The drawing conclusions can be listed as followed:

- 1) Built model that is equipped with half-infinite meshes successfully estimates the roughness parameters since they match well with experimental findings. It is demonstrated that the lowest value for difference percentage between numerical and experimental results appear to be around 8% for

Ra parameter. This result puts the study in a good position among the reference literature examined.

2) To eliminate the low-penetration effect that occurs in impacts of rectangular and triangular shot particles due to initial face contact, some amount of surface extension is introduced to these particles. The surface roughness results got enhanced in most of the cases. The best result in this condition is to be around 6% difference in Ra parameter between numerical and experimental findings.

3) A similar model that is equipped with Encastre boundary conditions instead of half-infinite mesh boundaries are introduced. The impact region is taken as 2.5 mm x 2.5 mm in this case. These simulations are run until 200% coverage. It is observed that, the results at 100% coverage level are mostly over acceptable difference percentage threshold. As the coverage increases to 200% with impacting another set, the final results are lowered and thus got closer to experimental findings. Coverage increase had a positive effect on the final values.

4) As the model with half-infinite meshes gave better matching results with experimental findings, it is decided to utilize this model instead of the model with Encastre boundary conditions. It is also observed that, extension mostly had good effect for matching the experimental findings unless the impact sequence is dominated by the presence of initially face-contact (i.e. rectangular or triangular) particles.

A further enhanced shot particle characterization possibly taking into account the dominance of rectangular shot particles could be a topic of possible improvement on the model. Another promising study would be testing the substrate material and evaluating the required material properties directly in order to input them to FEA model.

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Appendix

Table A.1: Abbreviations and full names of the Polymers

Abbreviation	Full Name
AES	Acrylonitrile Ethylene Styrene
ASA	Acrylonitrile styrene acrylate
PCTA	Polycyclohexylenedimethylene tere/isophthalate copolyester
PCTG	PolyCyclohexylenedimethylene Terephthalate glycol copolymer
PHA	Polyhydroxyalkanoates
PLA	Polylactic acid
SMA	Styrene maleic anhydride
TPU	Thermoplastic polyurethane
ABS	Acrylonitrile butadiene styrene
PC	Polycarbonate
PE	Polyethylene
PMMA	Polymethylmethacrylate
PP	Polypropylene
PTFE	Polytetrafluoroethylene
PVC	Polyvinyl Chloride
PVDF	Polyvinylidene fluoride
PEEK	Polyetheretherketone
POM	Polyoxymethylene

Cut-off = 0.25		Probe tip radius = 2 μm		All units are in μm				
PC-Alumina	Probe position (left-center-right)	Ra	Rq	Rz	Rmax	Rt		
68ar/150mm/3second/1-4	-3.75	3.51	4.07	15.95	18.34	19.59		
68ar/150mm/3second/1-3	-2.5	3.17	4.19	14.28	24.86	24.86		
68ar/150mm/3second/1-2	-1.25	4.14	5.13	19.03	22.86	23.96		
68ar/150mm/3second/1-1(center)	0	3.76	4.73	17.33	24.61	25.45		
68ar/150mm/3second/1-5	1.25	2.93	3.87	15.57	21.15	24.06		
68ar/150mm/3second/1-6	2.5	4.01	5.38	19.43	30.53	35.89		
68ar/150mm/3second/1-7	3.75	4	5.08	20.06	22.39	25.21		
Mean value		3.617143	4.631429	17.37857	23.53429	25.57429		

PC-Alumina	Probe position (left-center-right)	Ra	Rq	Rz	Rmax	Rt		
68ar/150mm/3second/2-4	-3.75	2.9	3.56	13.94	17.21	18.39		
68ar/150mm/3second/2-3	-2.5	4.06	5	18.95	21.49	25.05		
68ar/150mm/3second/2-2	-1.25	4.02	5.31	20.34	28.08	29.22		
68ar/150mm/3second/2-1(center)	0	2.96	3.72	15.11	15.93	16.7		
68ar/150mm/3second/2-5	1.25	3.49	4.38	15.75	21.99	21.99		
68ar/150mm/3second/2-6	2.5	3.08	3.98	15.35	23.12	23.38		
68ar/150mm/3second/2-7	3.75	2.68	3.67	13.96	22.77	25.66		
Mean value		3.107143	4.231429	16.34286	21.51286	22.91286		

PC-Alumina	Probe position (left-center-right)	Ra	Rq	Rz	Rmax	Rt		
68ar/150mm/3second/3-4	-3.75	3.21	4.19	15.58	17.2	23.36		
68ar/150mm/3second/3-3	-2.5	3.32	4.27	15.82	22.51	24.78		
68ar/150mm/3second/3-2	-1.25	4.26	5.31	20.01	25.38	27.03		
68ar/150mm/3second/3-1(center)	0	3.89	5.18	20.85	26.1	30.76		
68ar/150mm/3second/3-5	1.25	3.15	3.93	13.55	18.06	19.58		
68ar/150mm/3second/3-6	2.5	4.18	5.29	18.3	27.93	27.93		
68ar/150mm/3second/3-7	3.75	3.35	4.42	16.1	23.82	24.54		
Mean value		3.614286	4.655714	17.17286	23	25.6286		

Average results for 21 measurements		3.512857	4.50619	16.8981	22.68238	23.68133		
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Figure A.1: All experimental results with measured sections