Study of Volcanic Ash Impact onto Turbine Blades in Jet Engines

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Abstract

Gas turbines are of great importance in industry. In the turbine section within a jet engine, thermal barrier coatings (TBCs) are utilized to protect the metal turbine blades, thus improve the efficiency of engine. However, this coating is extremely vulnerable to attack by injected particulates. This ingested particulate is often referred to as "CMAS" (Calcia-Magnesia-Alumina-Silica). Among all the CMAS materials, Volcanic Ash (VA) is the most common type which aeroengines may encounter during the flight. This type of CMAS material would melt in the combustion section by ultra high temperature and then impact the turbine blades with relatively high speed. Some of the particles would then stick on and bond with the TBC, thus cause degradation of the protecting coating. In this way, the jet engine would be permanently damaged.

In the recent years, experiments have been done by different researchers to elaborate the effect of CMAS materials on TBCs. However, there is still a lack of knowledge in the bonding mechanism and physical adhesion between the CMAS particles (especially VA particles) and the substrate. A study of VA particle impingement is required in order to understand particle impingement, phase transition and heat transfer, bonding mechanism and splat morphology in detail.

In this research, experiments were carried at Cambridge University, by Prof. Trevor William Clyne, Dr. James Dean and Dr. Catalina Taltavull to reproduce the VA-substrate impingement in jet engine. A Vacuum Plasma Spray (VPS) system was utilized to create a high-temperature, high-velocity flow field. Different types of Volcanic Ashes (VAs) were introduced into the experimental set-up. Sticking rate, Scanning Electron microscope (SEM) micrographs of deposition morphology were examined and collected. Chapter 3 elaborates the details of this experiment set-up and data collected from the experiment. This experiment set-up is utilized by the author for building numerical models and the result of this experiment is used to validate the numerical models.

Three numerical models were built to perform a systematic study. Firstly in Chapter 4, a Computational Fluid Dynamic (CFD) model was created to simulate the steady-state of the VPS flow field. The Discrete Particle Method (DPM) model was then utilized to simulate the injection of volcanic ash particles. After calculating the BI number, non-isothermal effects within the ceramic particles were simulated by introducing the heat transfer function by a user-defined function (UDF). This model gives the temperature gradient within and velocity of the in-flight VA particles at any time during the spray. It is shown that small particles (diameter < 10 µm) would easily be melted and reach the iso-thermal state. However, these particles would be largely influenced by the flow field thus bypass the turbine blades. The large particles (diameter > 50 µm) would easily impact the turbine blades, but would remain unmelted due to the large grain size. It is concluded that VA particles with diameter of 15 µm to 40 µm are the most "dangerous" particles, because these particles have both
relatively high possibility to be melted, and high possibility to impact thus adhere on the substrate.

Second of all in Chapter 5, systematic study of Yttria-stabilized Zirconia (YSZ) particle impingement and deposition on stainless steel in thermal spray process has been performed. A Coupled Eulerian and Lagrangian model was developed. This model is contribute to simulate the process of semi-molten particle impact. By utilizing this model, both the large deformation of liquid part and the plastic deformation of the solid part could be extracted. One fully molten and two semi-molten(solid core with liquid shell and solid shell with liquid core) cases were studied. The results of the numerical model matches well with the experiment and analytical data. Interest parameters such as velocity, temperature, fraction of liquid part were varied. The contact area, splat morphology and local contact temperature were collected and studied. It is shown that, the larger the liquid fraction is, the larger the contact area would be. Moreover, effect of roughness of substrate is also studied. It is suggested that substrate roughness whose average asperity size is higher than the 1/10 of particle size is beneficial for adhesion.

Third of all in Chapter 6, in order to simulate the impact for high-viscosity glass-state ceramic particles, Smoothed Particle Hydrodynamic (SPH) model was built. For high/ultra viscosity cases, traditional CFD method and Finite Element Method (FEM) would be extremely slow. SPH model transfers the Eulerian equations into Lagrangian equations. By utilizing this method, computational resources could be saved, and high viscosity impact could be simulated. The SPH algorithm was coded and equations for heat transfer was introduced to simulate the solidification of liquid. Systematic study were performed by utilizing this model. Viscosity, contact angle, velocity of particles were varied. Contact area, splat morphology and solidification at the contact area were examined. It is shown that, large contact angle would result in large contact area. However, particles impingement with low viscosity and high contact angle could result in the break up of the particles. The similar phenomena could be seen in experiment - small particles have lower viscosity and are approaching the substrate with a large contact angle. Therefore, the deposition of these types of particles show an obvious evidence of break up and oblique impact.
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Chapter 1

Introduction

1.1 Background

Gas turbines are of prime importance in a range of industrial sectors, particularly for power generation and for propulsion of aircraft and marine craft. Ceramic coatings within such turbines represent the predominant area of their development, playing increasingly key roles in providing protection of metallic turbine blades components. The main material in industrial used to coat the turbines is yttria-stabilised zirconia (YSZ), offering chemical stability, low thermal conductivity and sufficient stiffness and strength. Large temperature gradient would generated within the Thermal Barrier Coating (TBC) layers. In this way, metallic parts are protected from over-heating and oxidation. Plasma spraying is widely used to produce such coatings, particularly for power plant turbines. There is a strong driver for expanding their usage in aeroengines, in which Electron Beam Physical Vapor Deposition (EB-PVD) coatings are often preferred (in view of their superior resistance to spallation), despite them offering less efficient thermal insulation and being more expensive to produce.

However, jet engines are quite vulnerable to attack by injected particulates. Much ingested particulate is often referred to as "CMAS" (Calcia-Magnesia-Alumina-Silica). These are the main ingredients of what might be regarded as a family of ceramic particulate matter. There has, of course, been concern about ingestion of volcanic ash (VA) into aeroengines. Numerous aviation accidents and incidents were reported during the last several decades, caused by VAs. For example, during the early 1980s, ash clouds spewing from Galunggung Volcano on Indonesia’s Java island, a British Airways flight lost power on all four engines. Another 747 encountered similar problems while flying through the ash clouds over Mt. Redbout, Alaska.
At least 10 Jumbo jets and 10 DC-10s suffered multiple engine failures in 1991 from VA from Mt. Pinatubo in the Philippines. The most remarkable VA impact to aviation would be the 2010 eruption of Iceland’s Eyjafjallajökull volcano. Over 300 airports in about 20 countries were closed in Europe. This resulted in massive impacts on air travel worldwide. Over 100,000 flights were cancelled in April 2010, affecting 7 million passengers, and resulting in 1.7 billion USD in lost revenue to airlines according to an analysis by Oxford Economics. Reference [1] documents 79 damaging ash/aircraft encounters. Twenty-six of those involved significant to very severe aircraft damage, including nine encounters where engine failure occurred during flight.

CMAS ingestion can damage aeroengines in multiple ways, such as erode turbine compressor blades, reducing their efficient, clogging air filters, blocking fuel nozzles, adhering and accumulating onto the turbine blades, etc. Figure 1.1 illustrates different types of damage VA can do to harm the aeroengines.

Despite so many types of damage VA could bring to aeroengines, the composition of VA is often such as to be most likely to promote severe degradation of ceramic coatings. It is known [2–18] that VA ingestion can damage such ceramic layers, particularly TBCs, mainly by promoting sintering and hence making them prone to spallation. Such degradation commonly arises when ingested particulate adheres to the coating and either creates a CMAS-rich outer layer or leads to diffusion into the coating of these oxides, along internal grain boundaries and free surfaces (pores). These oxides do not readily dissolve in the zirconia lattice, but tend to form vitreous phases at grain boundaries, where they accelerate sintering, particularly if significant levels of "liquid" are created. The performance of turbojet engines have been largely
improved since invented. The ultimate goal of this improvement is to reduce the sfc (specific fuel consumption) thus increase the engine efficiency. In other word, we would like to generate more thrust while consuming less fuel. In order to achieve this goal, a higher turbine entry temperature is required. However, this improvement of turbine entry temperature, on the other hand, would help melting CMAS material thus aggravate the deleterious effect of the injected.

Sintering of TBCs, with or without CMAS, leads to microstructural changes that raise the thermal conductivity and the stiffness, the former caused by growth of the inter-splat contact area and the latter by inter-splat locking and splat stiffening, due to microcrack healing. Coatings become more brittle and less strain-tolerant as sintering proceeds, making them prone to spallation (usually as a result of differential thermal contraction stresses set up during cooling) and also to erosive damage. It may be important to monitor, not only chemical composition (and hence melting point and potency for formation of vitreous grain boundary phases), but also the distributions of particle size and shape. This is likely to affect the "deposition efficiency" (proportion of incident particulate adhering after impact).

Besides CMAS, other species of ingested particulates include salt, particularly in marine environments, and sulphur. The degradation that these species induce can affect both unprotected metallic alloys and ceramic coatings.

From the background knowledge introduced above, it is of great importance to understand, from a detailed perspective, the trajectory, heat transfer, phase transition and deposition morphology of the ingested particulates. In this way, we could find out under what circumstance would the turbine blades been damaged by these particles. An EPSRC project (EP/K027530/1) is then established to mainly focus on the following topics:

- To study the impact and adhesion of ingested particles on substrates in the turbine area and establish the regimes (operating conditions, particle characteristics etc.) in which such adhesion is likely to occur.
- To explore the scope for using variants of conventional plasma spray process, notably Solution Precursor Plasma Spray (SPPS) and the overspraying of "scavenging" outer layers, in order to counter sintering effects within protective coatings (promoted by ingested species) and hence to improve their thermo-mechanical stability.
- To develop an improved understanding of how ingested species can degrade performance of ceramic coatings in gas turbines and identify effective measures to counter these effects.

Participants and collaborators of this project are, Prof. Sai Gu and Mr. Zihang Zhu, namely the author of this thesis, from University of Surrey, UK, Prof. Trevor William Clyne, Dr. James
Dean and Dr. Catalina Taltavull from University of Cambridge, UK and Dr. G Sivakumar from International Advanced Research Centre for Powder Metallurgy and New Material (ARCI), India. Prof. Bill Clyne’s group have substantial prior experience on thermo-mechanical characterization of coated systems on macro and nano scales. They are one of the best-known group for CMAS-related degradation of TBCs. ARCI is a leading group in the field of surface modification technologies, with history of technology development & transfer. They own large amount of unique coating facilities and have considerable processing expertise. Meanwhile, they are well-equipped for characterization and performance evaluation. Prof. Sai Gu’s group have substantial expertise in computational analysis of coating processes and have done considerable prior work on impact dynamics of various engineering phenomena. Workloads are distributed based on expertise of each collaborators. Experiments were designed and carried out in University of Cambridge. Chapter 3 would describe in details about this approach in order to help reader of the thesis to better understand the numerical model developed by the author in chapter 4, 5 and 6. Experiment data are then collected and distributed to Prof. Sai Gu’s Group. Numerical models were developed by the author based on the experiment setup in order to analyse and compare with the experimental results. Meanwhile, ARCI would try to improve the performance of protective ceramic coatings in gas turbine engines. The work of ARCI group will not be described in this thesis since it is not related to the work done by the author. Details of all the related works of the collaborators could be found on PROtection against Volcanic ash Induced Damage in Aeroengines (PROVIDA) website https://www.ccg.msm.cam.ac.uk/initiatives/provida/overview.

1.2 Aims and Objectives of this thesis

The thesis aims to improve understanding of the mechanisms, by which injected species and under what operating conditions, could volcanic ash adhere to the coatings by utilizing numerical modelling approach.

The objectives are:

- Partially participating in the experiment designed by Dr. James Dean and Dr. Catalina Taltavull and helping collect and analyse experimental data.
- Numerical modelling of the experiment, taking into consideration the non-isothermal effect for large VA particles, and validate with experiment data
- Numerical modelling of single particle impingement and study the deposition morphology systematically based on the model
Analysing the numerical results together with the experimental data, and identifying the regimes in which adhesion is likely to occur. Furthermore, identifying the most dangerous particle size and operating temperature.
1.3 Work Flow of Numerical Study

In the experiment designed and conducted by Dr. James Dean and Dr. Catalina Taltavull, a Vacuum Plasma Spray (VPS) was utilized as the heat source to replicate a jet engine turbine section. VPS would generate high-temperature and high-velocity flow and thermal field. By adjusting the volume flow rate of argon and hydrogen, the average velocity and temperature in the vacuum chamber can be altered. However, the temperature and status of the induced particles are the coupled effect of 1. the temperature of the flow field 2. the travel time of the particles 3. the size and property of the particles 4. the position of the substrate. The possible scenario of the particles travelling in the plasma jet could be seen in Chapter 4. The temperature would drop dramatically along the direction of the plasma jet. The temperature of the VA particles would increase initially and start to melt from the particles’ surface. Then, due to the temperature drop of the plasma jet, the VA particles would then cool down from the surface. Therefore, with different particle size or different position of substrate, the particle could be in different states (glass state, semi-molten state, molten state or solid state). In this case, the design of the experiment should be very accurate, in order to get the desired states of particles. For the above reasons, developing a numerical model would be more appropriate in case of observing states of particles. The whole numerical model could then be segmented into four parts.

1. A numerical model to calculate the steady flow field of the VPS (See Chapter 4 for details)
2. A numerical model to track the in-flight particles in the steady flow field (See Chapter 4 for details)
3. A numerical model to study the semi-molten particle impingement and phase transition (See Chapter 5 for details)
4. A numerical model to study the glass-state deformation (See Chapter 6 for details)

Figure 1.2 illustrate the diagram of the work flow.

Figure 1.2: Diagram of work flow for numerical work
Figure 1.3: SEM analysis of deposited volcanic ash

1.4 Contribution of This Work

1.4.1 Research Challenges and Related Contribution

There are three fundamental research challenges identified above: (1) Due to the low thermal conductivity of ceramic particles, temperature gradient would form within particles and it is complicated to determine the phase of particle before its impingement onto turbine blades. (2) In the semi-molten particle impingement scenario, former researchers normally treated the solid part as rigid body or a moving frame. However, the deformation of the solid part would largely influence the morphology and heat transfer of the liquid part. (3) In high-viscosity liquid impingement scenario, conventional Computational Fluid Dynamic (CFD) method requires large amount of computational resources and is very time-consuming. It is almost impossible to model the VA liquid impingement by utilizing the conventional CFD method, due to its high viscosity. In this thesis, a range of numerical models and techniques that address each of these challenges are reviewed and presented.

**Temperature gradient and status of in-flight particles.** It is quite complicated to measure the exact temperature and phase of VA in a high-velocity and high-temperature flow field. Therefore, a numerical model which can calculate these data is required. In addition, due to the low thermal conductivity and short travel time of VA particles in the temperature field, non-isothermal effect has to be taken into consideration for some particle. Moreover, with coupled effect of ambient temperature field, thermo-mechanical property of volcanic ash, and velocity of in-flight particles, particles would be in different phases before its impingement onto the blades. Figure 1.3 illustrates three types of VA depositions: unmelted(solid phase), softened/semi-molten, molten. Experimental done by Shinoda et al. [19] has shown, during the process of plasma spray, temperature gradient exists within ceramic particles.

In this thesis, the flow field is initially modelled by using conventional CFD method. The
injection of VA particles was then performed by utilizing a Lagrangian method: Discrete Phase Model (DPM). And heat transfer between the fluid phase and VA particle surface, as well as the intra-particle heat transfer is considered. Figure 1.4 illustrates the temperature gradient and phase transition of a VA particle travelling in a flow field at different position.

This computational model the author developed would help determine not only the exact velocity of VA particles before its impingement, but also the temperature gradient and phase. The results was then extracted and would be utilized as initial condition of single particle impingement case. Chapter 4 elaborates the principle of this model and demonstrates how it works.

**Deposition morphology of semi-molten droplet.** The results of the previous model shows that for medium-sized VA particulates, a large temperature gradient would present within the particles. As a result, these particles often impinge at the substrate in a semi-molten form; which in turn substantially affects the final characteristics of the morphology of deposition. As stated in the literature review, little modelling and simulation effort has been targeted towards its case due to the difficulties which arise when trying to model both solid and liquid phases. Previous modelling work [20–24] are all limited to implementing Volume of Fluid (VOF) approach. By utilizing VOF, the solid part behaves as a rigid body without considering any possible deformation of both particles and the substrate at impact. Therefore, error would occur while simulating the morphology and heat transfer between the particles and the substrate. This thesis introduced a novel modelling approach of a Coupled Eulerian and Lagrangian (CEL) method for both 3D
fully molten and semi-molten droplet impingement process. The simulation provides an insight to the deformation mechanism of ceramic particles and illustrates the freezing-induced break-up and spreading at the splat periphery.

Figure 1.5: Comparison between simulated (a) and experimental (b) YSZ droplet impinging onto a stainless steel substrate at temperature of 513K [25] (top view)

Figure 1.5 illustrates comparison between computational results from this thesis and experimental data [25] of molten ceramic droplet deposition.

Figure 1.6: Top view of splat morphology for semi-molten droplet impact with a core size of 40 $\mu$m respectively from numerical model

Figure 1.6 exemplifies the simulated results of semi-molten ceramic particle impingement by implementing CEL model. The plastic and elastic deformation on both substrate and particle’s solid part could be observed.
**High/Ultra viscosity liquid ceramics impingement.** The viscosity of the VA particle is dramatically depend on temperature. It could vary from 1 Pas to $10^9$ Pas. In the scenario of high or ultra viscosity droplet impingement, conventional CFD method based on Eularian mesh is very time consuming. In order to keep the solution stable, the timestep $t$ would keep decrease with the increase of the viscosity. This thesis implement a meshless Lagrangian method, Smoothed-particle hydrodynamics (SPH) to solve this. Figure 1.7 shows the comparison of VA particle splat morphology between the SEM micrograph and the result from SPH model.

![Comparison between SEM micrograph and SPH model](image)

Figure 1.7: Comparison between SEM micrograph of medium size Laki droplet with relatively high viscosity and the numerical model

### 1.4.2 Contribution

**To identify particles with high possibility to adhere.** Only considering the effect of VA particles size, small particles are easily melted but more possible to be carried away by the fluid phase. On contrast, large particles are less possible to be affected by fluid phase while are quite resistant to the temperature. This thesis concludes a range or particle size which is the most dangerous to the blades in the experiment. The particles within the size range are very likely to adhere to the blades thus cause degradation of ceramic layer. It is shown in Figure 1.8 that, with the growth of particle size, the chance of particle striking on the blade would increase. However, Decrease of the particle size helps the particle to melt in the combustion chamber. And melted
Figure 1.8: Diagram of dangerous particle size zone concluded from numerical model

Particle are more likely to adhere to the blades and cause more severe damage while unmelted ones can only result in plastic deformation. Chapter 4 explains how the conclusion is drawn.

**To improve the design of the experiment.** The aim of the experiment is trying to study the relationship between the characteristics of VA, i.e. particle size, composition, crystalline/amorphous content, glass transition temperature/melting temperature, and the adhesion rate of VA. This systematic study of the factors affecting adhesion of VA particles requires a set-up in which relevant parameters could be properly controlled. However, it is complicated to maintain VA particles in desired phase (melting), especially in a high-temperature, high-velocity flow field. Initially, the experiment was designed based on empirical data. However, with the development of the numerical model, a detailed flow field could be predicted. In this case, the experiment is optimised so that the target phase of VA particles could be reached and the systematic study could be carried on.
2.1 Introduction

As described in Chapter 1, the research areas of interest could be split into the following parts:

- Volcanic Ash injection into turbine section of jet engines.
- Failing mechanism of jet engine turbine coatings caused by injection of molten CMAS.
- Experimental and numerical study of Volcanic Ashes.
- Numerical modelling of jet engine turbine section.
- Numerical modelling of single particle impingement.
- State-of-art technology to prevent TBCs from CMAS attack.

The main research area of this study is, volcanic ash impingement in turbine section of jet engines. This topic only become critical for the recent years. Rather surprisingly, there appear to be very few reports [26] in the open literature of such experimental or numerical work with a gas turbine, although there is naturally quite extensive in-service experience and there have also been studies of deposition efficiencies using various test facilities [27–29]. Meanwhile, another research area - Thermal Barrier Coating (TBC) process is also of great interest. This is because TBC process itself is, to certain extends, identical to the scenario that Volcanic Ash (VA) particle impinge and stick onto the turbine blades. Both scenarios includes 1. Elevated ambient temperature 2. Relatively high impact velocity 3. Injected ceramic particle and 4. The parameters of interest are bonding mechanism, splat morphology and sticking rate. Therefore, research related TBC coating, especially numerical models, are also reviewed, and evaluated in this chapter. The study of the failing mechanism of turbine coatings caused by VA injection, as
well as study of VA particle itself is reviewed here. A insightful understanding of influence by the injected particulate could be given by these studies. This study could also benefit from existing modelling work of high-temperature, high-velocity flow field and of particle impingement field. These numerical models could be either utilized or improved to simulate the specific study - numerical modelling of volcanic ash particles’ impingement onto turbine blades in jet engine. Moreover, researches regarding new TBC technology which helps the turbines to resist the volcanic ash impact are also recapped in this chapter.

2.2 Related Work

2.2.1 Influence of VA injection into jet engine

Reference [26] is another study conducted by Prof. T.W. Clyne’s group in 2013 regarding the volcanic ash ingestion into jet engine. In this study, a small gas turbine engine was used in order to investigate the deposition behavior of ingested VA powder. The experiment set-up and schematic drawing could be find in Figure 2.1.

Two engine speeds (62,000 and 120,000 rpm) and four different particle size distributions of VA particles were used in the experiments, with average particle diameters of about 20, 50, 75, and 100mm. The powder had a $T_g$ value of the order of 600 °C, with a substantial amorphous content, and a melting temperature around 1100 °C. Figure 2.2 summarizes the damage characteristics
Figure 2.2: Damage level index as a function of the total amount of VA injected, for the four particle sizes, with an engine speed of 120,000 rpm [26]

exhibited after all of these runs. This figure indicates that more deposition occurred with the coarser particles (50 100 µm size), and that in all cases the deposition was progressive with continued injection of powder.

However, the conditions within such set-ups are likely to be different from those created during ingestion into a real gas turbine engine. Although the temperature are quite similar to that of a real jet engine, the size of the combustion chamber is not big enough to ensure all the particles are fully molten, as could happened in real engine. In this case, only coarse particles would adhere on turbine blades purely by inertial behaviour.

In the experiments conducted by Crosby et al. [28], four series of tests were performed in an accelerated deposition test facility to study the independent effects of particle size, gas temperature, and metal temperature on ash deposits from two candidate power turbine synfuels (coal and petcoke). The facility matches the gas temperature and velocity of modern first stage high pressure turbine vanes while accelerating the deposition process. Particle size was found to have a significant effect on capture efficiency with larger particles causing significant thermal barrier coating (TBC) spallation during a 4h accelerated test. In the second series of tests, particle deposition rate was found to decrease with decreasing gas temperature. The threshold gas temperature for deposition was approximately 960°C. In the third and fourth test series, impingement cooling was applied to the back side of the target coupon to simulate internal vane cooling. Capture efficiency was reduced with increasing mass flow of coolant air; however, at
Figure 2.3: (a) Side view of the setup and sessile drop method during rapid heating: the volcanic ash compact, which is placed outside the furnace (Position a), was rapidly moved into the hot zone (Position b) after the furnace was heated up to the desired temperature; subsequently, geometric parameters were tracked with time. (b) Sintering and subsequent spreading of molten volcanic ash droplets for experiments with $T_{\text{max}}$ of 1451 °C, represented by a series of photographs showing the melting of a 3mm volcanic ash compact [30].

low levels of cooling, the deposits attached more tenaciously to the TBC layer. Post exposure analyses of the third test series (scanning electron microscopy and X-ray spectroscopy) show decreasing TBC damage with increased cooling levels. The result of this experiment approach shows that larger and hotter particles are more likely to deposit and hotter surfaces are more successful in capturing impinging particulate. However, the particles used in this research are coal and petcoke which has higher thermal conductivity and different composition and melting point as volcanic ash.

Another interesting study was done by Song et al. [30]. This article presents experimental results of wetting under highly dynamic conditions by directly exposing volcanic ash to high temperatures (between 1039 and 1451 °C), designed to replicate the heating conditions experienced by the volcanic ash entering an operating jet engine. The present sessile drop experiments were performed using volcanic ash-sized particles, produced by crushing a much larger volcanic bomb sample from the 2010 eruption of Eyja-kull volcano, Iceland. The experiment set-up could be found in Figure 2.3.

This study quantified how rapidly volcanic ash may be expected to melt, coalesce, and spread during rapid heating to high temperatures, similar to those encountered within operating jet engines. This experiment also reveal fundamental similarities in the spreading behavior of molten volcanic ash and pure liquid at high temperatures despite their additional complexities. However,
in this article only static heating without considering momentum energy of VA particles. The initial impact velocity and angle could largely affect the final morphology of VA deposition. Thus could potentially affect the adhesion ratio. Moreover, the size of VA “particles” is too large compared with those can reach turbine section of jet engine.

2.2.2 Degradation of CMAS

Upon beginning this research, most research work related to the correlation of CMAS and TBC are focused on the area of coating damage after CMAS adhesion. Article [31] investigated the thermochemical aspects of the degradation phenomena using a model CMAS composition and 7YSZ grown by vapor deposition on alumina substrates. After isothermal treatments of 4h at 1200 °C to 1400 °C, it is found that CMAS rapidly penetrates the open structure of the coating as soon as melting occurs, whereupon the original 7YSZ dissolves in the CMAS and reprecipitates with a different morphology and composition that depends on the local melt chemistry. References [2–18] give an idea of how CMAS ingestion and adhesion would damage the ceramic layers. In [8]’s work, three important aspects of the mechanism are investigated: (a) The sub-surface delaminations always initiate at surface-connected vertical separations. (b) They are fully-infiltrated with CMAS. (c) They are strictly mode I (failure caused by interlaminar tension, also known as crack opening). A thermal shock analysis has been invoked to identify a critical infiltration thickness, above which delaminations are possible. Figure 2.4 briefs the possible penetration of CMAS melts into TBC column microstructures. This CMAS melts at \( \sim 1240 ^\circ\text{C} \) When the TBC surface exceeds this temperature, the excellent wetting characteristics of CMAS cause it to penetrate to a depth where the TBC temperature equals to the melting point of CMAS. Thereafter, upon cooling, it solidifies as a fully-dense domain. The modified thermo-mechanical properties of this region increase its susceptibility to spalling (cold shock delamination). The analysis also defines a characteristic depth beneath the surface at which the delaminations are most likely. The observations made on the airfoils are consistent with these two dimensions. A second mechanism has been explored as the potential cause of large spalled regions also observed on the airfoils. However, this observation is not possible to verify the mechanism.

Previous work also reported that sintering of TBCs will lead to microstructural changes that raise the thermal conductivity [7,32,33] and the stiffness [4,6,34–37], the former caused by growth of the inter-splat contact area [38,39] and the latter by inter-splat locking and splat stiffening, due to microcrack healing [36]. Coatings become more brittle and less strain-tolerant as sintering proceeds, making them prone to spallation (usually as a result of differential thermal contraction stresses set up during cooling) and also to erosive damage. It may be important to monitor, not only chemical composition (and hence melting point and potency for formation
Figure 2.4: A schematic of a CMAS layer that forms on the TBC and penetrates once it melts. This layer develops a large compressive stress upon cooling to ambient because of the expansion misfit with the substrate. A delamination may be induced near the base of the TBC if the energy release rate associated with the stress in the CMAS layer is high enough. [8]

of vitreous grain boundary phases), but also the distributions of particle size and shape. This is likely to affect the "deposition efficiency" (proportion of incident particulate adhering after impact).

The review paper [40] by Dr. Vijay Kumar has thoroughly investigated the failure mechanism of TBCs from the following 6 perspectives: (a) Degradation mechanisms of TBC system with property–microstructure relationship. (b) Sintering effects and the efficacy of nano-structured coatings. (c) TBC oxidation behavior and hot corrosion degradation mechanisms. (d) CMAS attack, erosion, impact damage and the countermeasures. (e) Interfacial degradation, lifetime modules, challenges and future research trends. Within section (d), authors elaborated different types and causes of degradation which could be induced by injection of CMAS. As stated, the sand or ash particles adhere on the hot TBC surface wherein these particle deposits change into
molten CMAS glass and cause coating degradation. The melting point of CMAS differs with the variation in their composition. While below the melting point, the particles rebound off the surface and may lead to erosive damages [49]. On the other hand, molten CMAS would adhere to and penetrate TBC by capillary action as a consequence of the microstructure and morphology of the TBCs [8]. With the columnar microstructure, EB-PVD coating are more resistance to particle impact as well as stresses developed due to thermal expansion. However, this columnar microstructure would, on the other hand, accelerate the penetration of molten CMAS. At the same time, the strain tolerance capability of EB-PVD is reduced due to the infiltration of molten CMAS and hence the structure is no longer able to reduce stresses [52, 53].

This review paper also concluded most investigations regarding interaction between YSZ TBCs and CMAS. Some articles [31, 52] show that the coating exposed to CMAS becomes depleted in yttrium, allowing tetragonal to monoclinic transformations and flow of zirconium in the CMAS melt. The TBC degradation is attributed to the wetting of the TBC by CMAS; YSZ dissolves in CMAS and re-precipitates with a varying composition and morphology. It was observed that the CMAS attack takes place at a very fast speed [31, 52, 55]. A critical infiltration thickness has been identified, above which the penetrated layer is liable to delamination and the delamination occurred just above BC and at the base of the CMAS infiltrated layer, for a failed stationary aero-engine component [56, 57]. A set of delamination maps developed by Evans and Hutchinson [52] are implemented by superimposing cooling trajectories. A minimum level of CMAS attack to cause damage has been estimated for EB-PVD coatings. YSZ coatings undergo significant porosity reduction and enhanced sintering shrinkages due to CMAS infiltration, which adversely affects the thermal insulation property of the TBCs [58]. Most of the works have been undertaken to examine the deterioration of the coatings on the real turbine blades, post their service [56, 57, 59].

Peng et al. [60] investigated the microstructure evolution of YSZ TBC, produced by EB-PVD, under simulated CMAS condition and thermo-chemical interactions between CMAS deposits and YSZ so as to understand the failure mechanism of TBC by CMAS attack. The results showed that the accelerated degradation of EB-PVD YSZ coatings occurred due to CMAS glass penetration into the YSZ layer along the inter-columnar gaps. An interaction zone of about 20 \( \mu \text{m} \) thickness was found in YSZ surface layer, post-heat treatment at 1250 \(^{\circ}\)C for 4h. The interaction zone was sufficiently depleted in yttrium and it was the mixture of CMAS and YSZ with equiaxed structure. Degradation of YSZ coating occurred by delamination cracking of YSZ layer, after 8 h heat treatment. This was attributed to the thermal expansion disparity between undamaged YSZ layer and the interaction zone, the phase transformation being unlike the traditional interfacial cracking at the YSZ/metallic bond coat. The vertical cracks as a result of tensile stresses due to sintering of EB-PVD TBCs, occurring during heat treatment. The phase transformation is another possible mechanism of CMAS attack. Phase transformation of \( \text{ZrO}_2 \) (tetragonal to monoclinic) is martensitic transformation, very quick, uncontrolled and accompanied by volume expansion (3–5%). Thus stress is generated in the ceramic coat and as and when this stress
is large enough, micro-cracks are generated. The places near the surface and vertical cracks are subjected to extensive CMAS corrosion and thus more phase transformation occurred in these regions, which cause micro-cracks. YSZ structure gets disrupted thereby deteriorating the integrity of TBCs due to the propagation of micro-cracks. Figure. 2.5 are illustrate the appear and propagation of vertical cracks of TBCs.

Chen et al. [61] investigated the mechanisms governing foreign object damage and erosion at the surface temperatures above 1200 °C during turbine operation. Three different domains based on particle size, velocity, temperature and coating composition were explored by quantitative modeling of the erosion and wear processes. Domain I represented impact conditions in which the projectile creates deep plastic/dense zones, while the impacting particles are sizable and have higher velocity. A threshold condition must be surpassed before bigger cracks are induced, when plastic zone is confined within the oxide. The typical impacts at 1150 °C do not go beyond the threshold and a denser layer is created in the absence of any delaminations. Domains II refers to the impact condition that produces comparatively shallow denser zones, by the impact of intermediate size particles. Domain III represents the condition when the coating reacts in an elastic manner, for small particle impact at lower temperatures. Thus this model identified domains in which three different mechanisms govern erosion and ascertained the microstructure
2.2.3 Study of Volcanic Ashes

In the report from [62], a general introduction into magma fragmentation processes during explosive volcanic eruptions is presented. Also, it described the evolution of the eruption of Eyjafjallajoekull, presented the possibilities of ground based in-situ and remote measurements and numerical model studies of volcanic ash.

In the study [95–97], equations are given to estimate density, viscosity and surface tension of CMAS materials. The empirical formula were concluded based on analysing hundreds different type of CMAS. The surface tension could be calculated as \( \gamma (mN/m) = 271.2 + 1.48 \times \text{mol}\% Li_2O - 2.22 \times \text{mol}\% K_2O - 3.43 \times \text{mol}\% Rb_2O + 1.96 \times \text{mol}\% MgO + 3.34 \times \text{mol}\% CaO + \).
1.28*mol%BaO + 3.32*mol%SrO + 2.68*mol%FeO + 2.92*mol%MnO − 1.38*mol%PbO − 2.86 * B₂O₃ + 3.47 * mol%Al₂O₃ − 24.5 * mol%MoO₃ [97]. The composition dependent density could be calculated as \( \rho (\text{g/cm}^3) = 74.42 * \text{mol%SiO}_2 + 0.75 * \text{mol%Al}_2\text{O}_3 + 0.01 * \text{mol%TiO}_2 + 0.16 * \text{mol%SO}_3 [95].

In Giordano’s work [127], model for predicting the non-Arrhenian temperature dependence of viscosity for naturally-occurring silicate melts at atmospheric pressure (10⁵ Pa) is concluded. See Equation 2.1 for temperature dependence of viscosity (\( \eta \)):

\[ \log \eta = A + B \frac{T(K)}{C} \]

where A is a constant independent of composition and B and C are adjustable parameters. Compositional dependence is ascribed to B and C as linear combinations of oxide components (mol%) and several multiplicative oxide cross-terms.

\[ B = \sum_{i=1}^{7} [b_i M_i] + \sum_{j=1}^{3} [b_{1j} (M_{11j} M_{21j})] \]

\[ C = \sum_{i=1}^{6} [c_i N_i] + [c_{11} (N_{11i} N_{21i})] \]

where the M’s and N’s are combinations of mol% oxides. Online calculator based on this model is available at https://www.eoas.ubc.ca/ krussell/VISCOSITY/grdViscosity.html

### 2.2.4 Numerical work of particle trajectory and impingement

Although the damage of the CMAS to the TBCs are well studied, the scenario of single VA particle impingement and bonding mechanism in micro scale has not been studied before. In reference [61] discussed before, Chen X. et al. also developed a numerical model in order to simulate the impact of CMAS solid particle’s impact onto columnar microstructure of EB-PVD TBCs. Figure 2.7 illustrate the stress propagation within columns with different initial conditions. However, this model is more focus on the elastic/plastic deformation of TBCs, as well as on solid particle impact. As stated above, the most dangerous CMAS phase would be molten or semi-molten. Therefore, this numerical model could only be used while modelling of EB-PVD microstructure is needed.

As to the numerical work of in-flight ceramic particles, Vardelle et al. [63] can predict the trajectory of particles while Zhao et al.’s model [64, 65] can also simulate the heat transfer between the fluid phase and particles. Furthermore, Zhao’s model provided a way of estimating the velocity and temperature at the exit of the plasma nozzle in VPS. Figure 2.8 shows the result of Zhao’s model. It could be seen that, in Zhao’s work, particles were all treated as iso-thermal bodies. However, due to the low thermal conductivity and relatively large grain size of ceramic
Figure 2.7: Typical evolution of the tensile stresses in the EB-PVD microstructure [61]

Figure 2.8: Variations of: (a) particle temperatures; and (b) particle velocities along the plasma jet axis with initial particle position [65]

materials (such as zirconia and VA), temperature gradient would exist within the particles. Experiment has shown that, for ceramic particles larger than $60 \mu m$, a semi-molten status would exist during the plasma spray process [25]. Therefore, with a large range of size distribution, volcanic ash would be in a form of unmelted, softened(semi-molten) or molten before impinging onto the turbine blades. In addition, oxidation [66–68] and evaporation [69] of in-flight particles have also been modelled and examined with zirconia or molybdenum particles. However, for volcanic ash in this experiment, after calculation the Biot Number, the non-isothermal effect and melting is of great interest (especially for large particles) rather than oxidation or evaporation.

As to the particle impingement model. A lot of previous works have been done on pure solid [71, 72], semi-molten [73–75], and fully molten [77] particle impingement. Li et al. [71] and Gu et al. [72]'s FEA model was developed to study the high velocity impingement process of solid particles and the bonding mechanism between the particle and substrate. By utilizing Johnson-Cook strain hardening, temperature softening plasticity model, the deformation and
stress of the solid metal particles could be captured. Tabbara et al. [73]’s work simulated a semi-molten ceramic droplet’s impact onto a solid substrate at a relatively low velocity. A temperature gradient was initialized in the model and the whole deformation of the liquid shell was captured. Alavi et al. [74] considered the influence of phase change after the impact. Also, the influence of the core size was examined in their works. Wu et al. [75]’s work demonstrated the partially melted YSZ particle impact at relatively high velocity from 100 to 200 m/s. However, the heat transfer effect was ignored in their works. All the previous contributions mentioned above utilized Volume of Fluid (VOF) approach. Although the morphology of the liquid deformation and even the heat transfer of the whole process could be simulated, the deformation of the solid core could not be obtained due to the fact that the solid core was defined as rigid body in all publications. However, according to Li et al. [131]’s work, ductile material will have ductile behavior under certain circumstance like high temperature or high pressure. In this case, modeling the solid part as a rigid body is far from reality. Therefore, a new method is needed to simulate both the liquid and the solid part of the particle so that the result could be more realistic. The significance of research on semi-molten ceramic impingement is the damage on the substrate and the effectiveness of coating. With a more accurate model, the coating performance estimation could be improved. Some of the numerical work of particle impingement could be seen in Figure 2.9.

For particle impingement with high initial velocity and viscosity, the traditional method is very time-consuming. The Smoothed Particle Hydrodynamics (SPH) method seems to be a proper solution to this problem. SPH is a meshfree particle method based on Lagrangian
formulation. It was first invented to solve astrophysical problems in three-dimensional open space [78, 79]. Further improvement of this method has been done by [80, 81]. The main difficulties of implementing the SPH method is choosing a suitable smoothing functions. [78] proposed the original smoothing function, [82–85] improved the function to make it more suitable for specific cases. Among all these functions, [82] is the most frequently used and [85] claimed to be more suitable for high velocity impact cases. [86] have implement the heat transfer function together with the N-S equation. However, this model is limited to 2D geometry. There is no known implementation of SPH method on VA particle impingement.

2.2.5 Improving the Degradation Resistance of TBC Caused by CMAS

Recent investigations in the area have included several [41–48, 50] aimed at exploring modifications to TBC composition and/or microstructure designed to mitigate the effect of degradation caused by CMAS / VA. These studies offer some grounds for optimism that the problem can be controlled, although no clearly effective scientific strategy has emerged so far. The most related work to new material of protected coating would be article [51]. In this paper, it concluded that APS TBC made of $Gd_2Zr_2O_7$ is extremely effective against the damage by molten fly ash deposits. The results show that lignite fly ash, which was a representative particulate impurity expected in syngas, when it contacts conventional APS 7YSZ TBCs at 1200 °C, penetrates the full thickness (200 µm) of TBC and destroys it completely. However, under identical conditions, APS $Gd_2Zr_2O_7$ TBCs are highly resistant as the molten lignite fly ash infiltrates only up to 25 percent of the coating thickness. The reduction in the damages to the TBC is attributed to the development of a stable impervious crystalline layer at the interface between the TBC and molten fly ash, thereby stops the piercing molten fly ash front. Fig. 2.10 shows the general mechanisms vide which APS $Gd_2Zr_2O_7$ TBCs counter the molten ash attack. However, compare with EBPVD thermal barrier coatings, APS is not so widely used for protecting the turbines of jet engines. Let alone the composition of molten fly ash is not quite similar to CMAS or, in our case, volcanic ash.

Darolia et al. [70]’s research observed that a modulated TBC structure can withstand impact damage better when compared to straight TBC columns, as shown in Figure 2.11. The superior performance of modulated TBC structure is attributed to the layers between each zone of orientation, which act as sites for deflection of the impact stress. This results in the removal of only the outer layer, instead of the entire coating. Thus, in the case of modulated structure, instead of the loss of entire coating thickness, only a thin single layer (<25µm) is sacrificed.
Figure 2.10: Schematic diagram of APS thermal barrier coatings (cross-sectional view), accompanying lignite fly ash deposits, prior and post-heat exposure, depicting the possible interactions: (a) 7YSZ and (b) $Gd_2Zr_2O_7$. Diagram not to the scale. [51]

Figure 2.11: Observations on field returned high pressure turbine blades from the same engine service show that modulated TBC structure is resistant to particle impact damage. [70]
Chapter 3

Methodology

3.1 Introduction

As part of this EPSRC (EP/K027530/1) project and as a fundamental input to the numerical work done by Mr. Zihang Zhu, namely the author of the thesis, a simple experiment set-up was designed by Prof. T.W. Clyne, Dr. James Dean and Dr. Catalina Taltavull from Cambridge University, in order to reproduce the scenario of VA impingement onto turbine blades in a jet engine. The experimental research is primarily done by Dr. James Dean and Dr. Catalina Taltavull. The author of the thesis has regularly helped with the experiment as well as analyse the results from the experiment. Also the author helped to optimize the experimental design by utilizing the numerical model built by the author. The design parameters of the experiment, such as VPS configuration, injected particle size and properties, are used as an input to create geometry and set-up boundary conditions for the numerical work described in the following chapters. The results from the experiment, such as sticking rate, SEM micrograph of VA particle splats, temperature and pressure measurement of the VPS chamber [87, 88] as well as result data shown in Appendix A, are utilized to validate the results of author’s numerical work. The design and rationale of this experiment is elaborated in the following section, in order to give readers of this thesis an overview of the basis, which the numerical models described in the following chapters are built upon.
3.2 Experiment

The scope of this experiment is to investigate the scenario of VA impingement onto turbine blades in a jet engine. Figure 3.1 illustrates the estimated temperature, velocity and pressure in a typical aero engine. Despite the complicated structure of engine, turbine section is of prime interest to this research. The first stage of high-pressure turbine would face temperature from 1500°F (820°C), up to 2500°F (1370°C) [89]. And the velocity of the flow field would vary from 100 m/s to 500 m/s. Injecting VA particles into the real engine is the most direct approach for this study. However, the disadvantages of this approach are also obvious - expensive and complicate. Therefore, in a Gordon Laboratory, University of Cambridge, a customized experiment set-up was built to conduct the systematic study. A Vacuum Plasma Spray (VPS) system has been used as a heat source. A stainless steel tube was mounted in the VPS chamber, in order to provide an environment simulating that of a combustion chamber. Thermocouples and Pitot tubes were placed to measure temperature and velocity. Chamber pressure, plasma power and powder feeder rate were adjusted as appropriate to examine the effect of different parameters. Subsection 3.2.1 describes the setup of the apparatus comprehensively. The conditions generated in such a system are not very close to those in the combustion chamber of a gas turbine, particularly in terms of gas pressure (which was well below one bar in these experiments, compared with up to 40 bar in a combustion chamber). However, a key objective is to study the sensitivity of the probability of adhesion to parameters such as particle temperature and velocity at impact. Such information, acquired via experiments of the type described here, can then be used to predict the behaviour under conditions in a real engine.

![Figure 3.1: Engine estimated temperature, velocity and pressure](image)

Four ashes have been obtained, from the volcanic eruptions at: (a) Laki (from the fissure erup-
tion of 1783-4 in south-central Iceland), (b) Eldgja (from the fissure eruption of 934, very close to Laki), (c) Hekla 4 - Hekla is a highly active strato-volcano located about 70 km south-west of Laki, which last erupted in 2000 - and (d) Askja 1875 - another active strato-volcano, located about 150 km north-east of Laki, which last erupted in 1961, for this research. The original VA material was obtained (via Dr. Margaret Hartley of University of Manchester). It was subjected to a grinding operation in a rotary mill and then sieved to give several selected ranges of size. Subsection 3.2.2 elaborates characterization of these particles, including chemical composition, phase constitutions, particle size distribution, thermo-mechanical properties, etc. Subsection 3.2.3 discuss the outcomes of the experiment, including the morphology of the particle splat, measurement of deposition rate etc. Apart from these, the temperature and velocity measurement of the experiments were collected. The measurement data and Scanning Electron Microscope (SEM) micrographs of the deposition are utilized as an input or validation to the computational model.

3.2.1 Experimental Setup

In the laboratory in Cambridge University, researchers are trying to reproduce a controllable fluid field which is similar to that in an combustion chamber in an jet engine. Meanwhile, VA particles are delivered into this flow field to simulate the particle impingement. In this systematic study, relevant parameters, particularly velocity and temperature field of the gas and the orientation of the substrate, requires to be properly controlled. Moreover, it is also very important to be able to measure the incident particles that adhere. There are evidently attractions in conducting this experiment on real jet engine or other gas turbines. However, the cost would be very expensive and the results would be quite complicated to measure and collect. Furthermore, since it is only the combustion chamber and turbine sector that we are interested in, a simplified set-up would be a better choice.

In the current work, a Vacuum Plasma Spray (VPS) system (PlasmaTechnik Unit with and F4 gun and 7mm nozzle) has been used, with chamber pressure, plasma power and powder feed rates adjusted as appropriate. Figure 3.2 gives an intuitive impression of the experiment set up. The experimental arrangement is depicted schematically in Figure 3.3. A 1000\(\text{mm}\) long stainless tube with 100\(\text{mm}\) diameter was mounted in the middle of the vacuum vessel as a initial set-up. A F4 plasma gun was placed in the centre at one end of the tube. The temperature and pressure field generated by this set-up is proved to be not enough to reach the environment of a common jet engine combustion chamber. A numerical model described in Chapter 4 was built based on this initial set-up. The geometry of the tube was then varied according to the systematic study of the numerical model. A tube with length of 550\(\text{mm}\) and 80\(\text{mm}\) was utilized as a final design and it provides an environment simulating (at least approximately) that of a
combustion chamber (1500° F at tube entrance). A W-type thermocouple was located at 175mm away from the plasma gun nozzle exit. Two K-type thermocouples were placed at 340mm and 500mm. Axial gas velocities were established using type L Pitot tubes (Kimo Instruments), placed at 350mm and 450mm from the nozzle. A 55mm * 35mm * 20mm rotatable stainless steel substrate was mounted at 450mm (see Figure 3.4). And the dimension of the inserts was 40mm * 20mm * 1.7mm. Measured temperature and velocity were used for setting up and validating numerical models. The more temperature and velocity data points measured in the experiment, the better could we validate the computational model. Although, the the horizontal distance of thermocouples and Pitot tube were fixed. The measuring probes could still move along the radius of the stainless steel tube. For the purpose of collecting more temperature and velocity data, 7 temperature data and 2 velocity of the flow field were measured by shifting every probes along the radius of the tube. Therefore, for each specific experiment test case, there are 21 temperature and 3 velocity measurements.

Figure 3.2: Experiment setup in Cambridge University
Figure 3.3: Schematic representation of the experimental set-up for monitoring of particle deposition rates, based on a plasma torch located within a vacuum chamber.

Figure 3.4: Geometry of rotatable substrate

Three different sets of VPS operating condition were employed (A B and C), as shown in Table 3.1. The coupled effect of increasing volume flow rate of argon and reducing the chamber pressure would result in an elevation of the average velocity and temperature of the flow field. In this way, parametric study regarding the temperature and velocity of flow field could be done. Figure 3.5 illustrates the arrangement of the ash feeder. VA particles were delivered in to the plasma jet through a long narrow pipe with an angle of 50°. The exist of the ash feeder was 40mm away from the plasma nozzle and the vertical distance between the pipe exit and centre of the plasma jet is 10mm. After the whole VPS system had stabilized under the selected operating conditions (usually takes around 30 seconds), VA particles were injected into the plasma jet through the ash feeder. The injection rate of VA was controlled at a predetermined rate (34.3mg/s) and the duration of injection was also standardized at 10 seconds. Thus the quantity of powder injected remained the same in all cases (343 ± 34mg, human error...
considered). Deposition rates were established by weighing the insert in the substrate before and after each experiment. The mass of an insert was about $11 - 12 \, \text{g}$ while the weigh gains after injection were of the order of $2 - 30 \, \text{mg}$. Although the mass change is relatively small compared to the overall insert mass (approximately 0.020.3%), the precision of the balance is $\pm 50 \, \mu\text{g}$ which is less than 10% of the mass gain, particularly for the higher deposition rate cases.

![Figure 3.5: Experimental arrangement of ash feeder](image)

The fraction of particles sticking on the insert was calculated based on the assumption, which is, the injected particles across the section of the tube were uniformly distributed. This assumption was checked by prolonged injection experiments in which substrate were placed at various locations in the section, using thermal conditions such that most particles could melt and then adhere to the substrates. In this way, this assumption was confirmed, at least toward the end of the tube, the particulates had become uniformly distributed throughout the cross-section. Therefore, the estimated weight of particles hitting substrate was calculated by the overall injected particle weight times ratio $f$. $f$ is a ratio between the area of tube cross-section and the projected area of insert at the flow direction (see equation 3.1 for details).

$$f = \frac{Lb\sin\theta}{\pi R^2}$$

(3.1)

Where $L$ and $b$ are the in-plane dimension of insert and $R$ is the inner radius of the tube. Since $L$ was 40mm, $b$ was 20mm and $R$ was 40mm in all test cases, with $\theta$ value of 90°, 60°, 30°,
corresponding value of $f$ are 15.9%, 13.8%, 7.96%. The deposition ration $f_{dep}$ was thus calculated by equation 3.2. Subsection 3.2.3 contains the detailed experiment data and calculation for every test cases.

$$f_{dep} = \frac{W_{increased}}{W_{inserted}} * f$$ (3.2)

### 3.2.2 VA Powder Characterization

Four types of ashes have been obtained, from the eruptions at: (a) Laki (from the fissure eruption of 1783-4 in south-central Iceland), (b) Eldgaja (from the fissure eruption of 934, very close to Laki), (c) Hekla 4 - Hekla is a highly active strato-volcano located about 70 km south-west of Laki, which last erupted in year 2000, and (d) Askja 1875 - another active strato-volcano, located about 150 km north-east of Laki, which last erupted in 1961. Details of these eruptions could be found in [91–94]. The as-received ash was ground in a rotary mill and then passed through sieves with spacing of representative size ($10 \mu m$ to $90 \mu m$). Figure 3.6 shows the SEM micrographs of the ground and sieved VA particles. As can be seen, the particles exhibit in a rather irregular morphology originally.

![SEM micrographs showing typical particle morphologies for the four types of ash: (a) Laki, (b) Eldgja, (c) Hekla and (d) Askja](image)

Figure 3.6: SEM micrographs showing typical particle morphologies for the four types of ash: (a) Laki, (b) Eldgja, (c) Hekla and (d) Askja
Table 3.2: Set of operating condition of VPS

<table>
<thead>
<tr>
<th>Composition (w%)</th>
<th>Laki</th>
<th>Hekla</th>
<th>Askja</th>
<th>Eldgja</th>
</tr>
</thead>
<tbody>
<tr>
<td>$SiO_2$</td>
<td>50</td>
<td>65</td>
<td>72</td>
<td>50</td>
</tr>
<tr>
<td>$TiO_2$</td>
<td>3.16</td>
<td>0.47</td>
<td>0.88</td>
<td>2.42</td>
</tr>
<tr>
<td>$Al_2O_3$</td>
<td>13.17</td>
<td>14.16</td>
<td>14.62</td>
<td>12.53</td>
</tr>
<tr>
<td>$FeO(T)$</td>
<td>14.32</td>
<td>5.67</td>
<td>3.79</td>
<td>15.32</td>
</tr>
<tr>
<td>$MnO$</td>
<td>0.22</td>
<td>0.22</td>
<td>0.09</td>
<td>0.23</td>
</tr>
<tr>
<td>$MgO$</td>
<td>5.17</td>
<td>0.14</td>
<td>0.82</td>
<td>5.64</td>
</tr>
<tr>
<td>$CaO$</td>
<td>10.17</td>
<td>3.42</td>
<td>2.44</td>
<td>10.44</td>
</tr>
<tr>
<td>$Na_2O$</td>
<td>2.82</td>
<td>4.8</td>
<td>3.51</td>
<td>2.64</td>
</tr>
<tr>
<td>$K_2O$</td>
<td>0.47</td>
<td>2.01</td>
<td>2.26</td>
<td>0.33</td>
</tr>
</tbody>
</table>

The chemical composition of the four types of VAs, obtained from EDX data, are shown in table 3.2. This table tells us that all four types of VAs have more or less similar composition, while Askja and Hekla are relatively rich in $Si$ (around 15%) but are less of other cations. This is broadly consistent with the concept of material from the Hekla and Askja eruptions being more viscous, since these (low valance) cations are known to act as “network-modifiers” in inorganic glasses, breaking up the linkages between the silica coordination octahedra and hence reducing the viscosity, whereas high silica glasses are expected to be more viscous. The higher contents of the divalent (Fe, Ca and Mg) ions in Laki and Eldgja are particularly noticeable.

The phase constitutions of these ashes were investigated using X-ray diffraction. The spectra are shown in Figure 3.7, together with indications of the phase proportions that they represent. It can be seen that both Hekla and Askja are fully amorphous, while the other two contain significant proportions of two crystalline phases.

![XRD spectra from the four ashes, with indications of the approximate glass contents](image)

Figure 3.7: XRD spectra from the four ashes, with indications of the approximate glass contents

The glass transition temperature and melting point of the VA were obtained with the set-up
shown in Figure 3.8 (a). A cold isostatic press was used to fabricate a cylindrical pellet of VA, about 5 mm in diameter and 1.5 mm in length. This specimen was placed in an alumina crucible and an alumina push rod applied a constant load of 0.3N to the specimen, which was heated at 5°C min⁻¹. Initially, the powder compact expands on heating, but then a contraction is observed. It is because the VAs are passing through the glass transition temperature $T_g$. As the amorphous fraction softens dramatically, so that powder particles start to deform and the compact becomes denser. The contraction accelerates when the particles finally melt at temperature $T_m$. Figure 3.8 (b) illustrates typical curves of dimensional change of the VAs. As can be seen, all of the glass transition temperature $T_g$ are in the approximate range 650 – 750°C, while $T_m$ is 1000 – 1100°C for Laki and Eldgja.

![Figure 3.8: Dilatometry data from the four ashes (as compacted powders), plotted as fractional length change, as a function of temperature](image)

In order to build numerical models to simulate the VA particles impingement, the thermo-properties of VAs are essential. However, due to the small size of VA particles, most properties could not be measured directly. Kucuk et al. [95], Giordano et al. [96] and Fluegel et al. [97] have related the density, viscosity and surface tension with VA chemical composition and temperature. Based on the equations mentioned in [95–97], the temperature and composition dependent density, viscosity and surface tension of all four types of VAs are calculated and shown in Chapter 6. The surface tension of Laki, Hekla, Askja and Eldgja at 1400°C are 388, 329, 320 and 391 mN/m respectively.
Table 3.3: Temperature of test case A (°C)

<table>
<thead>
<tr>
<th>Distance from the centre line (mm)</th>
<th>0</th>
<th>10</th>
<th>15</th>
<th>20</th>
<th>25</th>
<th>30</th>
<th>34</th>
</tr>
</thead>
<tbody>
<tr>
<td>Distance from the nozzle exit (mm)</td>
<td>175</td>
<td>1114</td>
<td>869</td>
<td>903</td>
<td>535</td>
<td>512</td>
<td>433</td>
</tr>
<tr>
<td></td>
<td>340</td>
<td>838</td>
<td>789</td>
<td>777</td>
<td>661</td>
<td>649</td>
<td>529</td>
</tr>
<tr>
<td></td>
<td>500</td>
<td>769</td>
<td>721</td>
<td>681</td>
<td>581</td>
<td>549</td>
<td>409</td>
</tr>
</tbody>
</table>

3.2.3 Experimental Results

For test case A, the typical temperature profile are shown in Table 3.3 below. As could be seen in this table, the temperature drops dramatically in both plasma jet direction and tube radius direction. The experiment results for test case B and C could be found in appendix A. The velocities measured at 355 mm and 455 mm away from the nozzle exit while there is no substrate mounted, is 92.19 m/s and 90.60 m/s. The velocity at 455 mm at the middle point along the tube radius direction, is 62.06 m/s and 87.77 m/s, without and with the substrate mounted. The introduction of substrate narrowed the fluid channel of plasma jet thus the velocity is increased. The deposition rate of all 4 different VAs with diameter of 25 μm with different temperature inputs (Case A, B and C) are shown in Figure 3.9. The horizontal axis of the graph is the measured temperature at the point of the substrate for each test cases. It is very clear that, the deposition rates increase dramatically with increase of temperature. For those particles with high glass transition temperature, exposing in an low-temperature environment results in almost 0% of deposition rate (Hekla and Askja at gas temperature of 800°C). The deposition rate of Eldgja and Laki are more or less the same, while are much higher than the other two types (Hekla and Askja).

Figure 3.9: Deposition rates of VA of particle size 25 μm with different temperature set-up
Figure 3.10 depicted the low magnification of deposited VA at different temperature (1\textsuperscript{st} and 3\textsuperscript{rd} rows), as well as SEM micrographs of VA splat morphology (2\textsuperscript{nd} and 4\textsuperscript{th} rows). These micrographs give a direct impression of the influence of temperature on deposition rate for different types of VAs. With the identical test condition (figures in same row in 3.10), Laki VA and Eldgja VA are more likely to deform and stick on substrate comparing with Hekla and Askja. This is related to 3.8, both Hekla VA and Askja VA have higher melting point than Laki VA and Eldgja VA. And also referring to 3.7 Laki VA and Eldgja VA contain less glass content than Hekla VA and Askja VA. With same VA type but different test cases (figures in same column in 3.10), the experiment results clearly show that with increasing of the temperature and velocity would result in higher deformation of VA particles as well as sticking rate.

Moreover, the coupled effect of particle size and temperature would also result in different splat morphology of VAs (see Figure 3.11).
More SEM micrographs of VA splat morphology (for different grain size, operating condition and type of VAs), are could be seen in later chapters and some of which would be utilized to validate the results of numerical work.
Chapter 4

Numerical study of in-flight CMAS particles

4.1 Introduction

As discussed in Chapter 3, the prerequisite for modelling deposition of VA particles is the capability of understanding and modelling both the particles’ trajectory and in-flight intra-particle heat transfer. Hereafter, pure solid [71, 72], semi-molten [73–76] or pure liquid [77, 118] particle impact model can then be adopted in order to simulate micro scale particle impact. Thus, the deposition morphology and contact area can be obtained. Hence, the rate of adhesion could be determined based on these computational models.

As to the numerical work of in-flight ceramic particles, Vardelle et al. [63] can predict the trajectory of particles while Zhao et al.’s model [64, 65] can also simulate the heat transfer between the fluid phase and particles. In Zhao’s work, particles were all treated as iso-thermal bodies. However, due to the low thermal conductivity and relatively large grain size of ceramic materials (such as zirconia and VA), temperature gradient would exist within the particles. Experiment has shown that, for ceramic particles larger than 60 μm, a semi-molten status would exist during the plasma spray process [25]. Therefore, with a large range of size distribution, volcanic ash would be in a form of unmelted, softened(semi-molten) or molten before impinging onto the turbine blades. In addition, oxidation [66–68] and evaporation [69] of in-flight particles have also been modelled and examined with zirconia or molybdenum particles. However, for volcanic ash in this experiment, the non-isothermal effect and melting is of great interest rather then oxidation or evaporation.
In this chapter, a comprehensive computational model to simulate the experimental set-up was described. The VA particle trajectory could then be simulated. An in-flight intra-particle heat transfer and phase transition model was coded and compiled. The numerical results were validated with the deposition morphology from the experiment. Furthermore, the most dangerous VA particle size is determined based on the numerical model.

4.2 Methods

A comprehensive numeric model was built to simulate the experiment set up. First of all, the VPS without an ash feeder or a substrate was modelled. A proper initial temperature and velocity estimation is needed at the exit of the nozzle (see section 4.2.2 for details). The static temperature and velocity fields were validated by the measurement points from the experiment. Second of all, the numerical model of the VPS with the substrate was built. Owing to the introduction of the substrate, the spray field was influenced and the new fields were compared with the experimental data. Third of all, the volcanic ash injection was modelled by utilizing DPM model. The trajectory and the residence time in high temperature of particles could then be obtained. Finally, the intra-particle heat transfer and phase transition model were coded and employed.

Therefore, the non-isothermal effect and phase transition for the in-flight particles at any point, including the very point before the impingement, could be obtained. Although, in the experiment, the intra-particle temperature gradient is difficult to be measured, especially for particles with high velocity. The numerical results can still be indirectly validated by comparing with the final morphology of ash deposition. The data extracted from this numerical work could be utilized to create a realistic boundary condition for micro-scale particle impact model for further research.

The commercial software, ANSYS FLUENT, was used for numerical work, a User Defined Function (UDF) was used for coding the heat transfer and phase transition.

4.2.1 Model Geometry

The geometry of the 3D numerical model was built based on the experiment set up. The meshes were refined at the place where large temperature and velocity gradient occurred, i.e. outlet of the nozzle, near the wall and area near the substrate. The exit of the nozzle was set as inlet, while the nozzle, stainless steel tube and vacuum chamber were defined as wall. Other areas which connect to the chamber were set as pressure outlet. Owing to the simplicity of the geometry, structured mesh was generated in order to increase stability and accuracy of the calculation. The 3D computational domain could be seen in Figure 4.1.
4.2.2 Modelling Static Fluid Field

In this work, VPS is utilized as a heat source to heat up and accelerate VA particles. Argon (Ar) is injected as primary gas while hydrogen ($H_2$) as secondary gas. An accurate numerical model of the static fluid field would help examine the flight trajectory of the VA particles as well as the inter-particle heat transfer. The general governing equations, Navier-Stokes (equation 4.1 in Cartesian coordinates) coupled with the Realizable $k - \epsilon$ turbulence model and energy model were utilized to model VPS system. Species mixture model was turned on to model mixed gas injection.

$$\frac{\partial}{\partial t} v + \nabla \cdot vv = -\frac{1}{\rho} \nabla p + \nu \nabla^2 v \tag{4.1}$$

Where $v$ is the fluid velocity vector in Cartesian Coordinate. $P$ is the fluid pressure, $\rho$ is the fluid density, and $\nabla$ indicates the gradient differential operator. $\nu$ is the kinematic viscosity, and $\nabla^2$ is the Laplacian operator.

According to Chang et al. [120], the following equations were used for drawing the profiles of temperature and axial component of velocity, at the nozzle exit.

$$T = (T_{max} - T_a)(1 - \left(\frac{r}{R}\right)^{4.5}) + T_a \tag{4.2}$$

$$u = (u_{max} - T_a)(1 - \left(\frac{r}{R}\right)^2) \tag{4.3}$$

where $T_{max}$ and $u_{max}$ are the velocity and temperature of the plasma jet at the nozzle exit. $T_a$, is the temperature of the anode, set to 700 K, and $R$ is the nozzle radius. Owing to the fact that the temperature and velocity of the plasma jet at the nozzle exit is too high to be measured, a reasonable estimation is needed in order to set up the initial boundary conditions. The energy
rate equilibrium model (equation 4.4) concluded by Zhao et al. [64] was utilized to estimate the initial temperature.

\[ \dot{E} = \dot{E}_i + \dot{E}_l + \dot{E}_h \]  
(4.4)

where \( \dot{E} \) is the energy input rate, \( \dot{E}_i \) is the energy loss rate to the plasma gun cooling water, \( \dot{E}_l \) is the dissociation and ionization energy consumption rate, and \( \dot{E}_h \) is the heating energy consumption rate.

Table 4.1: Gas properties and parameters used to calculate nozzle exit temperature and pressure [64, 87, 121, 122]

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molecular Weight (Ar)</td>
<td>39.948 kg/mol</td>
</tr>
<tr>
<td>Molecular Weight (H₂)</td>
<td>2.016 kg/mol</td>
</tr>
<tr>
<td>Specific Heat (Ar)</td>
<td>see equation 4.10</td>
</tr>
<tr>
<td>Specific Heat (H₂)</td>
<td>see equation 4.11</td>
</tr>
<tr>
<td>Thermal conductivity (Ar)</td>
<td>0.0158 W/(mK)</td>
</tr>
<tr>
<td>Thermal conductivity (H₂)</td>
<td>0.1672 W/(mK)</td>
</tr>
<tr>
<td>Viscosity (Ar)</td>
<td>1.58 \times 10^{-5} kg/(ms)</td>
</tr>
<tr>
<td>Viscosity (H₂)</td>
<td>8.4 \times 10^{-6} kg/(ms)</td>
</tr>
<tr>
<td>VPS current (I)</td>
<td>800 A</td>
</tr>
<tr>
<td>Chamber Pressure (P)</td>
<td>12000 Pa</td>
</tr>
<tr>
<td>Ar flow rate (F_{Ar})</td>
<td>50 L/min</td>
</tr>
<tr>
<td>H₂ flow rate (F_{H₂})</td>
<td>2 L/min</td>
</tr>
<tr>
<td>Gas constant (R)</td>
<td>8.31 J/Kmol</td>
</tr>
<tr>
<td>Q_{Ar}</td>
<td>1.5206 \times 10^6 J/mol</td>
</tr>
<tr>
<td>Q_{H}</td>
<td>1.3117 \times 10^6 J/mol</td>
</tr>
<tr>
<td>Q_{H₂}</td>
<td>4.320 \times 10^5 J/mol</td>
</tr>
<tr>
<td>K₁</td>
<td>413.3 (V s^{0.5})/mol</td>
</tr>
<tr>
<td>K₂</td>
<td>407.6 (V s^{0.5})/mol^{0.5}</td>
</tr>
<tr>
<td>K₃</td>
<td>17.39 V</td>
</tr>
<tr>
<td>k₁</td>
<td>0.032 Pa/K^{−2.5}</td>
</tr>
<tr>
<td>k_d</td>
<td>17.97 Pa/K^{−2.5}</td>
</tr>
</tbody>
</table>

It is proposed by Zhao et al. [64] that the terms on LHS and RHS of equation 4.4 could be expressed as:

\[ \dot{E} = I(K_1 F_{Ar} + K_2 \sqrt{F_{H₂}} + K_3) \]  
(4.5)

\[ \dot{E}_l = 0.54\dot{E} \]  
(4.6)

\[ \dot{E}_i = \chi_{Ar} Q_{Ar} + \chi_{H₂} F_{H₂} Q_{H₂} + 2\chi_H \chi_{H₂} F_{H₂} Q_H \]  
(4.7)

\[ \dot{E}_h = \int_{T_r}^{T} (F_{Ar} C_{Ar} + F_{H₂} C_{H₂}) dT \]  
(4.8)

where \( I \) is the plasma current, \( F_{Ar} \) is argon flow rate, \( F_{H₂} \) is hydrogen flow rate. \( Q_{Ar} \) and \( Q_H \) are the ionization energy of Ar and H, \( Q_{H₂} \) is the dissociation energy of \( H₂ \). \( K_1, K_2 \) and \( K_3 \) are constants. And these three values are mentioned in reference [64]. \( T_r \) is the room temperature.
which is set as 298 K, $T$ is the temperature of the plasma jet. $\chi_{\text{Ar}}$ and $\chi_{\text{H}}$ are the Ar and H degrees of ionization, $\chi_{\text{H}_2}$ is the $\text{H}_2$ degrees of dissociation. $\chi$ is calculated based on equation 4.9.

$$\frac{\chi^2}{1 - \chi^2} = \frac{kT^{2.5}}{P} e^{-Q/RT}$$

(4.9)

where, $k = k_i$ for all ionization, $k = k_d$ for $\text{H}_2$ dissociation, $P$ is the plasma gas pressure. $C_{\text{Ar}}$ and $C_{\text{H}_2}$ are the temperature-dependent specific heat of argon and hydrogen [121, 122].

$$C_{\text{Ar}} = 20.79 - 3.2 \times 10^{-5}T + 5.16 \times 10^{-8}T^2$$

(4.10)

$$C_{\text{H}_2} = 20.28 - 3.26 \times 10^{-3}T + 5 \times 10^4T^{-2}$$

(4.11)

Substituting equations 4.5, 4.6, 4.7 and 4.8 into equation 4.4. The temperature of the plasma was then iterated from 0 K to 20000 K with an interval of 0.1 K. The iteration was terminated and the estimated plasma jet temperature was calculated based on the criteria (equation 4.12).

$$\frac{|\dot{E} - \dot{E}_i + \dot{E}_i + \dot{E}_h|}{\dot{E}} \leq 0.01\%$$

(4.12)

The velocity of the gas is estimated based on Vardelle et al. [63].

$$u_{\text{max}} = 0.0259G^{0.21}I^{0.44}d_n^{-1.96}$$

(4.13)

where $G$ is the gas flow rate in kg/s.

Bring the parameters in table 5.1 in to equations above, the maximum temperature and velocity at the nozzle exit could be calculated. Result of the calculation could be seen in section 4.2.3. Plasma current $I$, chamber pressure $P$, argon flow rate $F_{\text{Ar}}$ and hydrogen flow rate $F_{\text{H}_2}$ is obtained from experiment set-up case A. The molecular weight, specific heat, thermal conductivity and viscosity are obtained from reference [121]. The $Q, K$ and $k$ constants for the two gases could be found in reference [64].

### 4.2.3 Modelling Particle Injection

After modelling the static fluid field, the VA particles injection was modelled by utilizing Discrete Phase Model (DPM). The DPM performs Lagrangian trajectory calculations for dispersed phases, including coupling with the continuous phase. With the lagrangian coordination, the Newton’s first law was employed on the particles by the force balance equation 4.14.

$$\frac{du_p}{dx} = F_D(u - u_p) + \frac{g_x(\rho_p - \rho)}{\rho_p}$$

(4.14)
where the parameters with subscript $p$ are the properties of the particle, while the ones without subscript are the properties of fluid phase. The first term on the RHS represents hydrodynamic force and $F_D$ could be expressed by:

$$F_D = \frac{18 \mu C_D Re}{\rho_p d_p^2}$$  \hspace{1cm} (4.15)

Here, $C_D$ is the drag coefficient and $Re$ is the relative Reynolds number.

The second term on the RHS is the force caused by gravity potential. In this case, due to the small size and high velocity of particles, the Froude number is much greater than 1. Hence, the particles are treated as aerosol and the influence of the gravity is therefore eliminated.

4.2.4 Modelling Intra-particle Heat Transfer

The Biot number ($Bi$) is a dimensionless quantity used in heat transfer calculations. $Bi$ gives a simple index of the ratio of the heat transfer resistances inside of and at the surface of a body. This ratio determines whether or not the temperatures inside a body will vary significantly in space, while the body heats or cools over time, from a thermal gradient applied to its surface. The equation for calculate $Bi$ could be find in 4.16:

$$Bi = \frac{L_c h_c}{k}$$  \hspace{1cm} (4.16)

where $L_c$ is the characteristic length, which in our case is related to the size of the volcanic ash particles. $h_c$ is thermal contact conductance and $k$ is thermal conductivity of the solid particle. The $h_c$ and $k$ could be found in table 4.3. With the particle diameter of 1 $\mu m$ to 90 $\mu m$, the $Bi$ number is calculated as from 0.022 to 1.65. The $Bi$ number of 25 $\mu m$ Laki particle is around 0.44.

In general, problems involving small Biot numbers (much smaller than 1) are thermally simple, due to uniform temperature fields inside the body. Biot numbers much larger than 1 signal more difficult problems due to non-isothermal effect in the solid itself. In this case, intra-particle heat transfer should be taken into consideration while calculating the heat transfer of VA particles.

The intra-particle heat transfer model utilized in this study is based on the work by Gu et al. [73, 123]. The heat transfer between the fluid phase and VA particle surface is determined by convection and radiation and the resulting heat transfer through the particle is calculated in spherical coordinates by equation 4.17, which includes the latent heat $H_f$, thermal conductivity $k$, specific heat $C_p$, solid phase temperature before melting $T_s$ and liquid phase temperature after melting $T_l$.

$$\frac{\partial T}{\partial r} = \frac{\alpha}{\Psi(T)} \left( \frac{\partial^2 T}{\partial r^2} + \frac{2 \partial T}{r \partial r} \right)$$  \hspace{1cm} (4.17)
where

\[ \Psi(T) = \begin{cases} 
1 + \frac{h_f}{c_p(T_l-T_s)} & \text{if } T_s \leq T \leq T_l \\
1 & \text{else} 
\end{cases} \]  

(4.18)

\[ \alpha = \frac{k}{\rho C_p} \]  

(4.19)

The boundary conditions at the particle surface and centre are defined in equations 4.20 and 4.21 respectively where the subscripts R and f represent the particle surface and continuous fluid phase.

\[ 4\pi R^2 k \frac{\partial T}{\partial r} \bigg|_{r=R} = 4\pi R^2 h_c(T_f-T_R) - 4\pi R^2 \epsilon \eta (T_R^4 - T_f^4) \]  

(4.20)

\[ \frac{\partial T}{\partial r} \bigg|_{r=0} = 0 \]  

(4.21)

where \( \epsilon \) is emissivity and is equal to 0.5 as recommended in [124,125]. \( \eta \) is the Stefan-Boltzmann Constant. \( h_c \) is the thermal contact conductance.

By using the Crank-Nicholson method, equation 4.17 and 4.20 could be discretized by \( N \) points, resulting in a form of equation 4.22 and 4.23.

\[ \alpha \frac{\Delta t}{\Delta r^2} (\Psi(i-1)T_{i-1} + (2\Psi_i + 2\alpha \frac{\Delta t}{\Delta r^2})T_i - \alpha \frac{\Delta t}{\Delta r^2} (i+1)T_{i+1} = \]

\[ \alpha \frac{\Delta t}{\Delta r^2} (1-i^{-1})T_{i-1} + (2\Psi_i + 2\alpha \frac{\Delta t}{\Delta r^2})T_i - \alpha \frac{\Delta t}{\Delta r^2} (i+1)T_{i+1}, i = 1, 2, \cdots, N-1 \]  

(4.22)

\[ -T_{N-1} + (1 - \frac{h_c \Delta r}{k_i})T_{N+1} = \frac{h_c \Delta r}{k_i} T_f - \frac{\epsilon \eta \Delta r}{k_i} [(T_{N-1})^4 - T_f^4] \]  

(4.23)

By applying theorem of L’Hospital, equation 4.21 is transformed into equation 4.24 and then discretized to equation 4.25.

\[ \frac{\partial T}{\partial t} = 3 \frac{\alpha}{\Psi(T)} \frac{\partial^2 T}{\partial r^2} \]  

(4.24)

\[ (\Psi^0 + 3\alpha \frac{\Delta t}{\Delta r})T_{0+1} - 3\alpha \frac{\Delta t}{\Delta r} T_{0+1} = (\Psi^0 - 3\alpha \frac{\Delta t}{\Delta r})T_0 - 3\alpha \frac{\Delta t}{\Delta r} T_{1+1} \]  

(4.25)

The discretized equations were then coded and compiled by FLUENT UDF. The simulation time step is \( 10^{-7} \) seconds and the particles are discretized into 20 points along the radius. The convergence criteria is set as \( 10^{-7} \). The simulated temperature profile for different particle size at different position could be seen in section 4.3.3.

### 4.2.5 Properties of Laki VA Particles

The mechanical and thermal-dynamic property of the Laki VA is of crucial importance for conducting the numerical simulation. Numerous work has been done on examining these
properties by other researchers. Kucuk et al. [126], Giordano et al. [127] and Fluegel et al. [128] have related the density, viscosity and surface tension with VA composition and temperature. A range of glass transition temperature and melting temperature has been measured by Taltavull et al. [87]. Table 4.2 shows the composition of Laki ash measured by Dr Taltavull in Cambridge University.

Table 4.2: Composition of Laki VA

<table>
<thead>
<tr>
<th>Composition</th>
<th>SiO$_2$</th>
<th>TiO$_2$</th>
<th>Al$_2$O$_3$</th>
<th>FeO</th>
<th>MnO</th>
</tr>
</thead>
<tbody>
<tr>
<td>Weight(%)</td>
<td>50</td>
<td>3.16</td>
<td>13.17</td>
<td>14.32</td>
<td>0.22</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Composition</th>
<th>MgO</th>
<th>CaO</th>
<th>Na$_2$O</th>
<th>K$_2$O</th>
</tr>
</thead>
<tbody>
<tr>
<td>Weight(%)</td>
<td>5.17</td>
<td>10.17</td>
<td>2.82</td>
<td>0.47</td>
</tr>
</tbody>
</table>

Table 4.3 illustrates the properties of the Laki VA used for the numerical work of this thesis. The surface tension and viscosity, though not needed for this work, could be very useful for the numerical work of single particle impingement [73, 76, 77].

Table 4.3: Laki VA properties [26, 77, 87, 126–128]

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density [87]</td>
<td>2000 kg/m$^3$</td>
</tr>
<tr>
<td>Specific Heat</td>
<td>$\sim 800$ J/(kgK)</td>
</tr>
<tr>
<td>Thermal conductivity</td>
<td>$\sim 2$ W/(mK)</td>
</tr>
<tr>
<td>Glass transition temperature</td>
<td>$\sim 875$ K</td>
</tr>
<tr>
<td>Melting temperature</td>
<td>$\sim 1300$ K</td>
</tr>
<tr>
<td>Latent Heat ($H_s$)</td>
<td>21000 J/kg</td>
</tr>
<tr>
<td>Thermal contact conductance ($h_c$)</td>
<td>220000 W/(m$^2$K)</td>
</tr>
<tr>
<td>Viscosity @ 1300 K</td>
<td>12655 Pa s</td>
</tr>
<tr>
<td>Surface tension</td>
<td>388 nN/m</td>
</tr>
</tbody>
</table>
4.3 Results

4.3.1 VPS Modelling Results

According to section 4.2.2, the temperature and velocity at the nozzle exit were calculated and initialized as $11800 \ K$ and $790 \ m/s$ respectively. The computational domain was filled with quiescent cold argon, which is then replaced by incoming plasma gas with elevated temperature, until a statistically steady state was reached.

Figure 4.2 illustrates the temperature and velocity contour for the plasma jet. Figure 4.2(a) briefs the plasma jet expended after spraying from the nozzle and the temperature drops dramatically from $11000 \ K$ to $5000 \ K$ within a distance of $40 \ mm$ along the jet direction. The plasma jet would further expended and the temperature would drop to less than $1000 \ K$ at $500 \ mm$ from the nozzle exit. Similarly, the velocity of the jet would drop dramatically from around $800 \ m/s$ to around $100 \ m/s$ at the position where the substrate is supposed to be installed (figure 4.2(b)).

Figure 4.2: Temperature and velocity contour for numerical model without substrate

Figure 4.3 compares the temperature extracted from the numerical model and measured during the experiment. It could obviously be seen that the temperature drops from around $1400 \ K$ to $1000 \ K$ at the centre line along the jet flow direction (from $175 \ mm$ to $500 \ mm$ away from the nozzle exit). Moreover, the temperature also reduces rapidly along the radius of the stainless steel tube. It is shown in both experimental and numerical results that the closer
the position is from the nozzle exit, the quicker the temperature would decrease along the tube radius. The temperature would all fall to around 450 $K$ near the stainless steel tube no matter how far the horizontal distance is from the nozzle exit. Owing to the expansion of the jet flow, the temperature drop along the tube radius would be more gentle with the increase of the horizontal distance from the nozzle.

Figure 4.3: Temperature comparison between numerical model and experiment data [87]

Figure 4.4 compares the velocity obtained from the numerical model and collected by pitot tube. It is shown that the velocity would decrease from around 90 $m/s$ at the center line to 60 $m/s$ at the center of the tube radius and further decay to 0 $m/s$ near the tube wall.

Figure 4.4: Velocity comparison between numerical model and experiment data [87]

A small distance could be seen between the experimental measurement and the numerical results. It could be caused by lacking of considering ionization, dissociation and recombination reaction. Since the plasma in this work is only used as a heat source, excessive detailed modelling of VPS is not necessary. Even so, the temperature and velocity field, especially the one at the centre of the plasma jet, matches well with the experimental data. The VA carried by the central
stream of the plasma jet is of prime interest because these are the ones who are most likely to impinge onto the substrate.

The validation of numerical results proved the estimation of initial temperature and velocity at the nozzle. The same settings were then utilized to perform the CFD simulation with the substrate installed at 455 mm away from the nozzle exit. Figure 4.5 demonstrates the temperature and velocity contour for the numerical model with introduction of substrate. As can be seen, the plasma jet elongates by around 5% due to the substrate. The ambient fluid temperature near the substrate surface would still be in a range of 750 K to 1250 K. In contrast, the velocity field is strongly influenced by the substrate. The fluid is stagnated near the substrate, while the velocity of the mixed gas bypassing the substrate is increased by 50%.

![Figure 4.5: Temperature and velocity contour for numeric model with substrate](image)

The introduction of substrate has forbidden the installation of the thermalcouples. For this reason, only the velocity at a single point between the substrate and the tube was measured by pitot tube. Figure 4.6 shows the comparison between the numerical results and experimental data point. As can been seen, owing to the block of the substrate, the fluid velocity is 0 m/s from the central to 15 mm along the radius. The velocity rockets to around 110 m/s and then decreases.
gently to 60 m/s with a distance of 20 mm, and further drops to 0 m/s near the tube wall. The numerical result is very close to the experimental data with an error of only 3.4%.

![Figure 4.6: Velocity comparison between numerical model and experiment data][87]

### 4.3.2 DPM Modelling Results

Whether the particle carried in the fluid will strike on or bypass the substrate is well-related to the Stokes number, which is a dimensionless number defined as below:

$$Stk = \frac{\rho_d d_d^2 u_0}{18 \eta_g l_0}$$  \hspace{1cm} (4.26)

where $\eta_g$ is the dynamic viscosity of the fluid phase, $u_0$ is the fluid velocity of the flow well away from the obstacle and $l_0$ is the characteristic dimension of the obstacle. $\rho_d$ and $d_d$ are the density and diameter of the particles respectively. When $Stk \gg 1$, impingement is expected, while $Stk \ll 1$ the particles will bypass the obstacles carried by the fluid stream. The critical diameter of the VA particles can then be calculated when $Stk = 1$, by rearranging equation 4.26.

$$d_{critical} = \sqrt{\frac{18 \eta_g l_0}{\rho_d u_0}}$$ \hspace{1cm} (4.27)

By substituting the parameters in equation 4.27, the critical diameter is calculated as 9 $\mu$m. Which means for Laki VA size far greater than 9 $\mu$m, it is more likely to strike on the substrate. The striking percentage against the particle size was studied based on this model. 100 particles with the diameter of 25 $\mu$m was injected in the numerical model as a benchmark. The diameter was then varied to representative values of 1 $\mu$m, 10 $\mu$m, 60 $\mu$m and 90 $\mu$m. The percentage of particles impacted onto the substrate was collected and demonstrated in table 4.4.

Figure 4.7 illustrate the velocity change for both impinged and bypassed particles of a (a) 25 $\mu$m and (b) 10 $\mu$m diameter, against the distance of flight path. For 25 $\mu$m particles, it is
clearly shown that, regardless of impinge or not, the particles would be accelerated by the plasma jet to around 110 m/s. The particles velocity would then either bottom to 0 m/s from 70 m/s if it hits the substrate, or keep decreasing to around 25 m/s if it travels around the obstacle.

By varying the particle size, the maximum velocity the particles could accelerate to and the initial velocity before impact would vary largely. Comparing with relatively small particles, large particles’ Stokes number is higher which means the behaviour of the particle is more likely to be dominated by inertia force. Therefore, these particles’ motion are difficult to be influenced by the fluid. Reversely, the velocity of the smaller particle is highly possible to be affected by the fluid phase. As shown in figure 4.7(b), according to the numerical results, the particles of 10 µm diameter would be accelerated to 130 m/s (which is 18.2 % higher than the one with a diameter of 25 µm). However, the velocity would reduced to 55 m/s (which is 21.4 % lower than the benchmark value) right before impingement. Moreover, the velocity of the small particle (≤ 10 µm) fluctuates more easily than larger particles (figure 4.7(b)). It also proves the theory.
Intra-particle Heat Transfer Modelling Results

The discretized heat transfer and phase transition equations were coded and utilized to observe the intra-particle thermodynamic status in the numerical model. According to the numerical results from section 4.3.1, the temperature drops dramatically from the nozzle exit along the plasma jet direction. Figure 4.8 briefs the possible forms of a VA particle travelling in the plasma jet before impact. As can be seen from the diagram, since the Laki VA particles were injected by the feeder with a room temperature, the surface of particles would be heated up by the elevated ambient temperature firstly. The whole particle would then be fully molten due to the ambient temperature is well above the melting point. If the substrate is installed close to the nozzle, a well-melted VA is expected to impact onto the substrate. However, if the substrate is installed far away from the nozzle, with the further decrease of the temperature, the VA particles would start to turn back to the unmelted form.

![Figure 4.8: Schematic diagram of in-flight particles heat transfer and phase transition](image)

Apart from the substrate installation position, the size of the VA particles also have a great impact on the final form right before impact. In terms of large particles, due to the size and low exposure time in elevated-temperature plasma jet, the energy would be insufficient to fully melt or partially melt the VA particles. Therefore, the VA particulate would be in a form of softened (semi-molten) or unmelted before impinge onto the substrate.

The spherical particle was discretized by 20 points along its radius, a typical particle temperature profile against the distance from the nozzle exit of a 25 \( \mu m \) Laki VA with the substrate installed at 455 \( mm \) away from the nozzle, is plotted in figure 4.9. Figure 4.9(a) illustrate the initial condition of the particles. All VAs would be preheated to 313 K to avoid any bonding or
attaching due to humidity. Figure 4.9(b) shows the surface of the particles starts to be heated by the plasma jet. The melting process could be seen in figure 4.9(c). The outer layer of the particles has melted while the core part of the particles is still absorbing energy to complete fusion without changing the temperature. The particles are then fully melted and the temperature starts to raise again, and reaches a pseudo iso-thermal states (almost no temperature gradient) right before impact (figure 4.9(d)). And also the flow field temperature drop could be seen in figure 4.9(e).

Figure 4.9: Non-isothermal effect of in-flight VA particles
The model was then performed on 25 µm, 60 µm and 90 µm particles with the substrate positioned at 455 mm and 900 mm away from the plasma torch. The final temperature profile before impingement for different particle size could be seen in figure 4.10. Figure 4.10 (a) and (b) shows that, wherever the substrate is, the 25 µm VA would all be fully melted and reaches a pseudo iso-thermal status before impact onto the substrate. With the growth of the particle size, figure 4.10 (c) and (d) indicates 60 µm particles also reaches a pseudo iso-thermal status with the temperature a little below the melting point. This means the 60 µm particles is in a deformable glass form which is very close to the molten liquid. For large particles (90 µm), the heat generated by the plasma torch is not enough to raise the temperature of the particles to the melting point. Therefore, these large particles are still in a form of solid/unmelted (figure 4.10 (e) and (f)). The BI number of 90 µm particle is around 1.65, therefore, a strong non-isothermal effect is expected and could be seen in large particles. In contrast, 25 µm particle’s BI number is around 0.44, and the numerical also shows only very small temperature gradient (∼ 0.50.6%) could be seen. comparing with large particles (∼ 38%)

With the further decrease of temperature (move the substrate backwards), the final temperature before impact of each particles would decrease due to the decrease of the ambient jet temperature.
The impact is transient so that the temperature gradient and phase transition is impossible to be measured during the experiment. Even so, the numerical model could still be validated by the morphology of the particle deposition. Figure 4.11 illustrates the Scanning Electron Microscope (SEM) analysis of the deposited Laki volcanic ash with different characteristic size (25 µm, 60 µm and 90 µm). Figure 4.11(a) shows, for 25 µm particles, the deposition is well-flattened and presents a mark of droplet impact. Figure 4.11(b) presents a morphology of 60 µm particle. The deposition is not as flattened as 25 µm but a round shape is beginning to form due to the surface tension of the melting particle. It is because the particle’s final iso-thermal temperature
is around the melting point. In that case, the 60 µm particles would be in a partially molten or at least softened form before the impact. On the other hand, the results of 90 µm particle deposition tells an obvious story. Figure 4.11(c) shows the deposition still maintains the grain shape of a solid VA particle, which means the heat of the plasma jet is not high enough to melt such a large particle. The results of the numerical model was then proved indirectly by the experimental results.

![SEM analysis of the deposited Laki volcanic ash of (a) 25 µm, (b) 60 µm and (c) 90 µm](image)

**Figure 4.11:** SEM analysis of the deposited Laki volcanic ash of (a) 25 µm, (b) 60 µm and (c) 90 µm

### 4.3.4 Most Dangerous Particle Size

From the numerical results of section 4.3.2, the very small particles (≤ 1 µm) have low possibility of striking on the substrate. In a jet engine, instead of striking on and adhere to the turbine blades, the very small particles would flow through the channel between the turbines. These particles would then accumulate and block the intake and air holes hence damage the engine in another way. In contrast, from section 4.3.3, very large particles (≥ 70 µm) would not be melted while impact onto the substrate. In this case, despite the high striking rate, these particles would more likely to bounce back instead of adhere on the substrate during impingement [87]. Due to the high stiffness of the TBCs, plastic damage generated by large particle impact is ignored.

Therefore, the small and medium particles would be more likely to both strike on and adhere
to the substrate, thus seriously damage the TBCs. Figure 4.12 concludes the findings from this numerical model. The red curve is the fitting line from table 4.4, which shows the increment of striking rate while increasing the size of the particles. The two blue vertical dotted lines show the separation size between molten, semi-molten and unmelted phase for particles. According to our assumption, the fully-molten particle with high striking rate would have higher possibility to stick on substrate and thus cause further damage to TBCs. The most dangerous particle size, concluded by the numerical study, is around 15 µm to 40 µm (shadow area in figure 4.12). For the particles whose size are within this range, the striking rate is above 50% while they are in a molten form. The experiment shows the similar results as the numerical outcomes. The adhesion rate of small and medium Laki particles could be 100% to 200% higher than the large ones [87]. Also, according to an non-confidential report by Rolls-Royce, the most critical VA particle size is around 5 µm to 20µm [98].

4.4 Discussion and Conclusion

In this chapter, a customized set-up was used to reproduce the scenario of volcanic ash impingement onto turbine blades in jet engine. The vacuum plasma spray was utilized as a heat source to heat up and deliver the volcanic ash particles. A numerical model was built to (a) model the VPS system (b) model the ash feeding (c) model the non-isothermal effect and phase transition of in-flight particles. The temperature field of (a) is extracted and compared with the
experiment data. It is shown in both experimental and numerical work that the temperature near the impact area is around 750 to 1250 K, while the velocity is around 75 to 100 m/s. It is well-established in numerical model (b) that, for the Laki particles whose size is greater than the critical diameter (9 µm), they are more likely to impact onto the substrate (98 % striking rate for 90 µm particles). Meanwhile, the small ones would fly around the obstacles (1 % striking rate for 1 µm particles). Numerical model (c) denotes detailed heat transfer and phase transition within the particle itself. Based on the numerical study, the small ones (25 µm) would firstly be heated and then melted, and reaches an iso-thermal condition of around 1350 K. Moreover, medium particles (60 µm) would be heated up and reach the temperature around the melting point(1300 K). In addition to this, large particles (90 µm) would remain its original shape since the heat of the plasma jet could not melt the grain. A large temperature gradient could be seen for large grain-sized particles. The numerical model (c) is then validated indirectly by the morphology of the particle deposition obtained from the experiment. Combining the results from (b) and (c) concluded that, ~ 15 – 40 µm would be the most dangerous particle size, because these particles have relatively high striking rate and are easily to be melted at the same time.

Improvement could be made by a more detailed VPS model as well as considering the non-spherical effect of VA particles during flight. A detailed VPS model considering ionization and recombination would help generating a more accurate spray field. Furthermore, considering the phase-dependent non-spherical effect (introducing non-spherical factor while the particle is in solid form) could help predicting the trajectory of particles more precisely (by considering a more accurate drag force).
Chapter 5

Numerical study of particle impingement by utilizing CEL method

5.1 Introduction

With the particulates’ velocity and temperature extracted from the computational model in Chapter 4, a microscopic computational model is needed for the multiphase particle impact scenario. Most numerical models for particle impingement were developed in the area of thermal spray or cold spray, for the reason that these coating process would include elevated temperature, high speed impact as well as small particle size and phase transition. The whole thermal spray process is identical to the experimental set-up built in University of Cambridge. Moreover, the research on the particle impingement in thermal spray has been studied for some years and lots of experimental data could be accessed in case of validating the numerical model. Therefore, Yttria-stabilized Zirconia(YSZ) particles is utilized to develop the microscopic impingement model in this chapter. Both YSZ and VA have high melting point, ceramic component and identical thermal conductivities.

Thermal spray is a coating technology on the basis of high-speed impact dynamics. During this process, the micro-sized or nano-sized spray particles are heated and melted by the hot gases and accelerated towards a target substrate surface. Melted particles would then impinge onto the coated target or onto one another. The splat will then splash, cool and solidify. In this way, a lamellar layer of coating is built up. According to [129, 130], the deformation of these particles is influenced by several particle parameters, including: velocity, particle size, particle melt fraction, particle and substrate material properties etc. Thermal plasma spray is commonly
utilized to deposit oxide ceramics such as Yttria-stabilized Zirconia (YSZ) in the size range of 20 µm - 90 µm [129, 130]. Based on the initial size of coating powder, some of them will be fully melted before hitting the substrate. Meanwhile some others, according to experiments [25], whose size is larger than 60 µm, would contain an unmelted solid core in the spray particle due to the high plasma temperature and low conductivity of ceramic powders. In this case, a large temperature gradient would exist along the radius of the particulate.

A lot of previous works have been done on pure solid [71, 72], semi-molten [73–75], and fully molten [77] particle impingement. Li et al. [71] and Gu et al. [72]’s FEA model was developed to study the high velocity impingement process of solid particles and the bonding mechanism between the particle and substrate. By utilizing Johnson-Cook strain hardening, temperature softening plasticity model, the deformation and stress of the solid metal particles could be captured. Tabbara et al [73]’s work simulated a semi-molten ceramic droplet’s impact onto a solid substrate at a relatively low velocity. A temperature gradient was initialized in the model and the whole deformation of the liquid shell was captured. Alavi et al. [74] considered the influence of phase change after the impact. Also, the influence of the core size was examined in their works. Wu et al. [75]’s work demonstrated the partially melted YSZ particle impact at relatively high velocity from 100 to 200 m/s. However, the heat transfer effect was ignored in their works. All the previous contributions mentioned above utilized Volume of Fluid (VOF) approach. Although the morphology of the liquid deformation and even the heat transfer of the whole process could be simulated, the deformation of the solid core could not be obtained due to the fact that the solid core was defined as rigid body in all publications. However, according to Li et al. [131]’s work, ductile material will have ductile behaviour under certain circumstance like high temperature or high pressure. In this case, modelling the solid core as a rigid body is far from reality. Therefore, a new method is needed to simulate both the liquid and the solid part of the particle so that the result could be more realistic. The significance of research on semi-molten ceramic impingement is the damage on the substrate and the effectiveness of coating. With a more accurate model, the coating performance estimation could be improved.

A Coupled Eulerian and Lagrangian (CEL) approach is utilized in this chapter to capture both the splash deposit of the liquid ceramic shell, and the deformation of the solid core and substrate. The 3D study particularly examines the single-particle impingement, liquid spreading, and solidification during the process. The result gives an insight of the morphology of fully molten ceramic particles impact and an idea of the phenomenon for semi-molten ceramic particle impact. The flattening degree of the particles are obtained and compared with both experimental and analytical data.
5.2 Numerical Method

The impacting behavior of both fully molten and semi-molten particle was modelled by using CEL approach. Due to the nature of Lagrangian method, it is always been used to simulate the solid mechanics problem. However, large deformation of the lagrangian part leads to extremely distorted elements and bad quality meshes, thus loses the fidelity of the results. In Eulerian analysis, an Eulerian reference mesh, which remains undistorted and unchanged during the whole simulation, is needed, to trace the motion of the particles. The advantage of an Eulerian formulation is that no element distortions occur. Disadvantageously, the interface between two parts cannot be described as precise as if an Eulerian formulation is used. Numerical diffusion can happen during the simulation. Also, a large computational domain needs to be generated in order to capture all the possible location which contains the material during the whole process. Therefore, plenty of computing resources are needed. A Coupled Eulerian-Lagrangian (CEL) method attempts to capture the strength of the Lagrangian and the Eulerian method. For general geotechnical problems, a Lagrangian mesh is used to discretize structures, while an Eulerian mesh is used to capture the volumetric motion of the particles and also some large distorted structure [132].

The Navier-Stokes equations govern all the fluid flow. Comparing to the traditional CFD methods, the CEL method introduces incompressibility, viscosity, etc via material law and properties and the governing equations are more general than Navier-Stokes equations. CEL is brute force implementation for CFD. No simplifying assumptions as well as structured mesh are needed for the CEL method [133].

5.2.1 Model Development

Two general types of models are generated in order to perform both molten and semi-molten ceramic particle impingement. Vardelle et al. [129]’s work illustrates the distribution of particle size, velocity and temperature of the particles in a typical plasma spray process. The experiment shows that the mean particle diameter measured was 30 $\mu$m, with an average velocity of 190 m/s before impact. In this case, a 30 $\mu$m, with an initial velocity of 190 m/s YSZ droplet was generated as a benchmark in this chapter. Owing to the axisymmetric characteristic of normal impact process, a 1/4 fully molten particle (shown in Figure 5.1(a)) with a diameter of 30 $\mu$m and an impact velocity of 190 m/s was created as a benchmark. For reducing the element number and also the computing time, a 70 $\mu$m $\times$ 70 $\mu$m $\times$ 20 $\mu$m stainless steel substrate was generated. The impact velocity was then varied from 100 m/s to 240 m/s and the flattening degrees were obtained. The influence of the impact velocity on the flattening degree were examined and compared with both the experimental data and the analytical results. Experimental results [25] present that particles whose diameter is greater than 60 $\mu$m had unmelted cores or shells. In this case, models of 1/4 80 $\mu$m sphere particle with a solid core of different sizes were created. The
computational model and mesh of semi-molten particle can be seen in Figure 5.1(b). However, due to the fact that the contact algorithm in CEL method is limited and the fact that the surface tension effect is not included in the material definition. Also, temperature cooling effect of the surrounding gas is not considered in this case. There will be some slight error in this simulation compared with the experiment data.

Figure 5.1: (a) Computational model of molten particle impact benchmark (b) Computational model of semi-molten particle impact with a core diameter of 60 $\mu m$. 
Table 5.1: Material properties

<table>
<thead>
<tr>
<th>Impinging droplet material</th>
<th>YSZ</th>
</tr>
</thead>
<tbody>
<tr>
<td>Substrate material</td>
<td>Stainless Steel(SS)</td>
</tr>
<tr>
<td>Substrate initial temperature</td>
<td>423 K</td>
</tr>
<tr>
<td>Solidus temperature(YSZ)</td>
<td>2799 K</td>
</tr>
<tr>
<td>Liquidus temperature(YSZ)</td>
<td>2801 K</td>
</tr>
<tr>
<td>Thermal conductivity (liquid YSZ)</td>
<td>2.00 W/(mK)</td>
</tr>
<tr>
<td>Thermal conductivity (solid YSZ)</td>
<td>2.32 W/(mK)</td>
</tr>
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<td>Thermal conductivity (SS)</td>
<td>14.9 W/(mK)</td>
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<td>Density (solid YSZ)</td>
<td>5890 kg/m²</td>
</tr>
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<td>Density (SS)</td>
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</tr>
<tr>
<td>Specific heat capacity (solid YSZ)</td>
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</tr>
<tr>
<td>Specific heat capacity (SS)</td>
<td>477 J/(kgK)</td>
</tr>
<tr>
<td>Thermal conductance</td>
<td>$5 \times 10^7$ W/(m²K)</td>
</tr>
</tbody>
</table>

5.2.2 Material Properties

The method for modelling the liquidus YSZ, Stainless Steel substrate, temperature profile and thermal and flow models are outlined below. The thermal-physical properties of the materials presented in this chapter are summarized in Table 5.1.

Mie-Grüneisen Equations of State

The thermodynamic behaviour model of real materials can be characterized by the following two-terms relations [134]:

\[ e(V, T) = e_{ref}(V) + e_T(V, T) \]  
\[ p(V, T) = p_{ref}(V) + \frac{\Gamma(V)}{V} e_T(V, T) \]  

(5.1)

(5.2)

Where \( V = 1/\rho \) denotes the specific volume, \( T \) denotes the temperature, \( p \) is the pressure, \( e \) is the internal energy, and \( \Gamma \) is the Grüneisen parameter which represents the thermal pressure from a set of vibrating atoms. The \( p \) and \( e \) with subscription \( ref \) represent the pressure and internal energy at a reference state usually assumed to be the state at which the temperature is 0K.

Combining equations 5.1 and 5.2, the most common form of Mie-Grüneisen equation of states could be obtained [135, 136]:

\[ p - p_H = \frac{\Gamma}{V}(E_m - E_H) \]  

(5.3)
Where $p_H$ and $E_H$ are the Hugoniot pressure and specific energy, the Mie-Grüneisen parameter $\Gamma$ is defined as
\[
\Gamma = \Gamma_0 \frac{\rho_0}{\rho}
\]  
(5.4)

Where $\Gamma_0$ is a material constant and $\rho_0$ is the reference density. The Hugoniot energy, $E_H$, is related to the Hugoniot pressure by:
\[
E_H = \frac{p_H \eta}{2\rho_0}
\]  
(5.5)

Where $\eta = 1 - \rho/\rho_0$ is the nominal volumetric compressive strain. Elimination of $\Gamma$ and $E_H$ from equation 5.3 yields:
\[
p = p_H(1 - \frac{\Gamma_0 \eta}{2}) + \Gamma_0 \rho_0 E_m
\]  
(5.6)

The Mie-Grüneisen equations of state represent coupled equations for pressure and internal energy. Solver solves these equations simultaneously at each material point by using explicit method.

**Linear $u_s - u_p$ Hugoniot Form**

In the absence of pronounced dynamic yielding effects or phase transitions, the hydrostatic pressure is commonly expressed by the Mie-Grüneisen equations of state (equation 5.3) together with a linear fit assumption for the shock velocity as a function of the particle velocity [137], i.e.,
\[
u_s = c_0 + s u_p
\]  
(5.7)

where $u_s$ represents the shock velocity, $c_0$ is the zero-pressure isentropic speed of sound, $u_p$ is the velocity of the particle, $s$ is a dimensionless parameter which is related to the pressure derivative of the isentropic bulk modulus. The speed of sound ($c_0$) of the fluid is inversely proportional to the fluid’s compressibility and also to the stable time increment when simulating. With the $u_s - u_p$ equation, the linear $u_s - u_p$ Hugoniot form is then written as
\[
p = \frac{\rho_0 c_0^2 \eta}{(1 - s\eta)^2} (1 - \frac{\Gamma_0 \eta}{2}) + \Gamma_0 \rho_0 E_m
\]  
(5.8)

The limitation of the compression parameters are given by $\eta_{lim} = 1/s$. In this project, the speed of sound of liquid YSZ was set as 3000 m/s and the dimensionless parameter $s$ was chosen as 2.39 as illustrated in [138, 139].

**Temperature-dependent Viscosity**

Due to the low conductivity of YSZ material, there will be a temperature gradient along the radius of the sphere particle. The particle in simulation was then assigned with a initial temperature gradient as shown in Figure 5.2. The temperature will maintain the same from the surface of solid core towards the centre. The particle temperature model was developed by Tabbara [73] and will not be described here. Furthermore, due to the low thermal resistance [129] and large
temperature gap between the particle and the substrate, a large temperature gradient would be
generated after the contact between the particle and the substrate. As a result, the viscosity will
differ from place to place due to the large temperature gradient. This will affect the flow and
energy dissipation of the liquid. Some research [129, 140, 141] has been done related to the
high temperature viscosity of the YSZ. Fantassi et al. [140] assumed a constant viscosity of
0.04 Pa·s, while Vardelle et al. [129] summarized an equation to calculate the viscosity of YSZ
at different temperature:
\[ \mu = 0.1 e^{\frac{5993}{T} - 2.95} \]  
(5.9)
Shinoda et al. [141] proved Equation 5.9’s behavior. Therefore, in this project, equation 5.9 was
utilized to calculate the viscosity of YSZ at different temperature.

![Temperature profile of liquid particle](image1)

(a)

![Temperature profile of semi-molten particle](image2)

(b)

Figure 5.2: (a) Initial temperature profile of liquid particle. (b) Initial temperature profile of
semi-molten particle with a core diameter of 40 \( \mu m \)

**Plastic Deformation of Solid YSZ**

Ceramic materials under normal pressure and temperature behave like brittle material. The
material fails as long as the stress reaches the fracture stress right after elastic deformation.
However, Brittle ceramics may become ductile above a specific temperature, which is referred to
as brittle-to-ductile transition temperature (BDTT). Below BDTT catastrophic fracture occurs
by crack propagation in bursting mode where as above BDTT, a certain amount of plastic
deformation can be obtained prior to the eventual failure. Moreover, some ceramics exhibit
superplasticity with an elongation rate exceeding 300%, at temperatures high enough above
their BDTTs [142–144]. Therefore, the ceramic core, in the semi-molten simulation, could
not be modeled as a pure brittle material since the whole impact process was conducted under
relatively high temperature (almost its melting temperature). Thus, certain high-temperature
plasticity attributes of YSZ should be defined for the ceramic core in order to visualize the plastic
deformation. The stress-strain curve from [145] was used to model the plasticity of the YSZ
ceramic core for semi-molten impact case.
Johnson-Cook Plasticity Model

The elastic response of the material follows a linear elasticity model, which is adequate for most impact cases. The plastic response of stainless steel is assumed to comply with the widely used Johnson-Cook plasticity model [146, 147] as follows:

$$\sigma = (A + B\epsilon_p^n)(1 + C \ln \dot{\epsilon}^*)(1 - (T^*)^m)$$  \hspace{1cm} (5.10)

Where $A$, $B$, $n$, $C$ and $m$ are material-dependent constants such as static yield strength, strain-hardening exponent, strain-hardening modulus, strain-rate-sensitive coefficient, and thermal-softening exponent. $\epsilon_p$ is the effective plastic strain. $\dot{\epsilon}^*$ is the effective plastic strain rate normalized with respect to a reference strain rate $\dot{\epsilon}_p/\dot{\epsilon}_0$. $T^*$ is defined as the following:

$$T^* = \begin{cases} 
0 & \text{for } T < T_r \\
\frac{T - T_r}{T_m - T_r} & \text{for } T_r \leq T \leq T_m \\
1 & \text{for } T > T_m 
\end{cases}$$ \hspace{1cm} (5.11)

Where $T_m$ is the melting point and $T_r$ is the reference or transition temperature. Since stainless steel is widely used metal, the Johnson-cook parameters is easily obtained by experiments and then tested in simulations.

5.3 Results

The following sections would illustrate the results of the computational model and the comparison with experimental data. Subsection 5.3.1 shows the utilization of CEL model in fully molten particle impingement. Subsection 5.3.2 shows the results in semi-molten particle (liquid shell and solid core) impingement while subsection 5.3.2 examined the effect of interested parameters during impingement for semi-molten particles with solid shell and liquid core.

5.3.1 Fully-molten Particle Impingement

The computational method was applied by simulating a 30 $\mu m$ fully molten YSZ droplet impinging onto a stainless steel substrate with an initial velocity of 190 $m/s$, using a dynamic temperature coupled explicit solver. Detail of this model are fully described in [129]. The simulation was stopped at 0.5 $\mu s$ as stated in [129]. Figure 5.3 illustrates the morphology of the impingement both in simulation and experiment [25]. The simulation result shows some splashes around the edge of the flattened droplet and a thicker part in the center of the splat which agree well with the experimental results. During the impingement process, the temperature drops dramatically within the contact area which led to an increase of the viscosity. The energy was then dissipated in the viscosity, the flow in the low temperature area was slowed down and formed a thicker part in the center of the splat. Figure 5.4 briefs the morphology of the whole
impingement process, the first column shows the top view while the second presents the side view.

Figure 5.3: Comparison between simulated (a) and experimental (b) YSZ droplet impinging onto a SS substrate at temperature of 513K [25] (top view)

The velocity of the impact was then varied from 100 m/s to 240 m/s to examine the influence of the velocity on the flattening degree. The experimental data were extracted from [129], shown in Figure 5.5 with black dots. When neglecting the contribution of the splat rim on the splat morphology, an analytical model developed by Pasandideh-Fard [148] describes the particle’s flattening degree $\xi$ is related to the droplet’s diameter $d$, kinematic viscosity $\nu$ and the impinging speed $V$ with the following form:

$$\xi = \frac{1}{2} \left( \frac{Vd}{\nu} \right)^{1/4}$$

(5.12)
Figure 5.4: 30 µm particle impingement process (scale bar represents 50 µm)
Figure 5.5 illustrates the flattening degree obtained from experiment, from analytical equation and from simulation. Although the experimental splats seem to be randomly spread, a clear trend can be seen from the data that the flattening degree is proportional to the impact velocity. Also, Equation 5.12 implies that the spread factor $\xi$ is proportional to $V^{1/4}$. The results of the simulation give a trend which matches well the experimental and analytical data.

![Figure 5.5: Comparison among simulated, experimentally measured [129] and analytical calculated [148] flattening degree for the molten YSZ droplet impinging at 190 m/s](image)

The energy during the whole impingement was tracked. The results illustrated that the kinetic energy of the droplet decreased and dissipated in the plastic strain of the substrate as well as the viscosity. Therefore, the deformation of the centre node on the contact surface of the substrate was examined and shown in Figure 5.6. As can be seen from the displacement-time figure, though small, increasing the impact velocity will increase the plastic deformation on the stainless steel on the substrate. Moreover, the influence will become greater when undertaking a high initial velocity. Using initial impact velocity of 80 m/s as a datum, the impact velocity was increased by 25%, 88%, 138%, and 300% while the final equivalent plastic strain on the substrate increased by 50%, 210%, 330%, and 680% respectively. This is due to with an elevated initial velocity, the whole system will contain more energy. Therefore, during the impact process, more energy was transferred and stored by the plastic deformation of the substrate. Furthermore, according to Johnson-Cook model, the high temperature in the centre part of the impact will soften the stainless steel thus relatively large plastic strain can be obtained in the centre of the contact surface than other nodes.
5.3.2 Semi-molten Particle Impingement

Particles with Molten Shell and Solid Core

The computational method was then applied by simulating an 80 µm semi-molten YSZ droplet impinging onto a stainless steel substrate with an initial velocity of 190 m/s. According to Equation 5.12, the degree of flattening $\xi$ will increase when increasing the size of the particle. However, experiments [25] shows that for particles whose size is greater than 60 µm, the flattening degree will actually decrease while increasing the particle size (shown in Figure 5.7).
Figure 5.8: 80 $\mu m$ semi-molten YSZ particle with 40 $\mu m$ solid core impingement process (scale bar represents 100 $\mu m$)
This is because, for large coating particles, the heat will not be enough to melt the particles thoroughly before its hitting the substrate. The same discussion and result could also be seen in Chapter 4 (large particle has relatively large internal temperature gradient and is hard to be melted). In this case, a solid core will remain in the centre of the particle. Due to the fact that a solid would not have a deformation as large as liquid, the flattening degree will actually decrease as shown in the experiment. The whole process of the impingement is shown in Figure 5.8 (80 µm YSZ semi-molten droplet with core size of 40 µm). As illustrated in the figure, during the whole process, the solid core will firstly impinge with the liquid shell. Then, the solid part will penetrate the liquid and hit the substrate, deform and bond. It is shown that, in the centre part of the contact surface, some of the shell part will remain at the bottom of the core. It is due to the heat exchange between the liquid shell and the substrate freeze the centre part of the liquid. Thus, the temperature of this part decrease which then makes the liquid part solidify and bond with the substrate. Several other semi-molten droplet impingement cases were then performed with core size ranging from 20 µm to 60 µm. The final deformation of the solid core and the morphology of the splat can be seen in Figure 5.9.

The flattening degree was collected and was shown in Figure 5.10. Comparing the flattening degree of the simulation with the experimental results in Figure 5.7, the semi-molten flattening degree is approximately 3.1 which can be seen in both experimental and computational results(with 0% to 25% solid core volume fraction). Furthermore, with the increase of the core volume fraction, the flattening degree will decrease dramatically. Also, as shown in Figure 5.9, the deformation of the core tends to decrease with the shrinkage of the core size. It can be seen from the figure that, the larger the core is, the more flatten the core will be. The top part of the sphere core remain undeformed while the bottom part start to deform. Normalizing the deformation with the core size, the maximum deformation factor was dropped from 0.252 to 0.110 then to 0.036. This gives a result that the liquid break-up of the liquid shell absorb the energy of the impact. The thicker the shell is, the more impact energy it is going to absorb, thus the smaller plastic deformation the solid core will end up with.
Figure 5.9: Deformation of the solid core and top view of splat morphology for semi-molten droplet impact with a core size of $60 \mu m$, $40 \mu m$, and $20 \mu m$, respectively.

Figure 5.10: The effect of core volume fraction on flattening degree, $\xi$. 

Particles with Solid Shell and Molten Core

This numerical model was then applied to another semi-molten particle impact scenario. Considering the place of the stainless steel substrate is placed far away from the plasma nozzle. The YSZ coating particles may initially fully melted. Then, due to the dramatic drop of ambient temperature, the heat would transferred from at the surface of the particles. Therefore, prior to the impingement, the surface of the particles would start to solidify while the core of the particle remain in liquid status. During the impact period, the kinetic energy of the particles would induce a large plastic deformation on both substrate and particle itself. Thus temperature would increased at the very point of contact.

A systematic study was conducted by utilizing the model developed. Several parameters of interest were studied, which include the radius of the particle $R_{\text{particle}}$, the radius of the crater on the substrate $R_{\text{crater}}$, depth of the crater $D_{\text{crater}}$, maximum temperature on substrate and on particle $T_{\text{max},\text{particle}}$ and $T_{\text{max},\text{substrate}}$. Normalized parameters were utilized in order to eliminate the influence of the magnitude. $NR_{\text{crater}} = R_{\text{crater}}/R_{\text{particle}}$ and $ND_{\text{crater}} = D_{\text{crater}}/R_{\text{particle}}$ were introduced and studied. Figure 5.11 illustrates the definition of each parameters.

Three parameters were studied systematically: 1. The diameter of the particle was 80 $\mu$m, the diameter of the liquid core was 40 $\mu$m, the velocity was varied from 50 m/s to 400 m/s

2. The diameter of the particle was 80 $\mu$m, the velocity of the particle was 150 m/s, the diameter of the liquid core was varied from 10 $\mu$m to 70 $\mu$m

3. The velocity of the particle was 150 m/s, the diameter of the liquid core was 50% of the diameter of the large particle, the diameter of particle was varied from 20 $\mu$m to 70 $\mu$m
The results of case 1 could be seen in Figure 5.12. It is shown that, with higher initial velocity, higher kinetic energy the particles would have. And more kinetic energy would be transferred into heat and then the temperature on both particle and substrate would increase (by around 100 K). Meanwhile, the contact area and depth of crater will increase along with the increase of velocity. Plastic deformation of the particle would be large and the particle would be flatter with the increase of velocity.

Figure 5.12: Velocities influence on \( N_{\text{crater}} \), \( N_{\text{D_crater}} \) and maximum temperature on substrate and particle.

The results of case 2 is shown in Figure 5.13. With little liquid core, the deformation on the particle would not vary too much. However, with large fraction of liquid part, the particles become more deformable. In this case, the maximum temperature on the particle would remain almost the same while there is little unmelted part in the core. Furthermore, a thin solid shell would lead to a large contact area, which would accelerate the heat transfer between the particle and the substrate. On the contrast, the plastic deformation on the substrate would decrease with an impact of a more "soften" particle.
Figure 5.13: Influence of fraction of liquid core on $NR_{crater}$, $ND_{crater}$ and maximum temperature on substrate and particle.

The results of case 3 is shown in Figure 5.14. It could be seen that, although the values of $R_{crater}$ and $D_{crater}$ were decreased with the decrease of the particle’s diameter, the normalized value $NR_{crater}$ and $ND_{crater}$ won’t change. The maximum temperature on the substrate and particles remains the same for this case.

Figure 5.14: Influence of particle size on $NR_{crater}$, $ND_{crater}$ and maximum temperature on substrate and particle.
5.3.3 Effect of Substrate’s Roughness

Mechanical bonding is observed in the coatings; hence, surface adhesion is believed to play an important role in the particle impingement and bonding. Nano/micro-scale material mixing and mechanical interlocking were identified and used to explain the enhancement of interfacial bonding. Mechanical anchorage, physical adhesion and metallic interactions are involved in all kinds of interfacial reactions. Thus, it is believed that rougher coating surface causes higher mechanical anchorage. High contact pressures are believed to be necessary conditions for particle/substrate and particle/pre-deposited material bonding. The contact pressure at the interface is strongly related to contact area and kinetic energy of particle. The impact of single particle of various materials on flat substrate surfaces for different velocities was modelled by using this FEA model. Many authors indicated that particle conditions prior to impact, such as particle velocity, temperature, and particle impacting angles will influence the deformation behaviours of particles.

Substrate roughness effect was investigated by several groups experimentally. In the section, the effect of substrate roughness on the deposition and deformation of particle has been studied through modelling of realistic grid blasted substrates. This section presents the study to examining the bonding mechanism particle impingement on roughened substrates and to establishing a correlation between spraying parameters and substrate morphology on resulting particle/substrate adhesion.

For ceramic materials, the deformation is relatively small comparing with metallic materials. And ceramic particles would be more brittle rather than plastic during impact. Therefore, in this study, copper particles and aluminium substrate was utilized for the systematic study. Smoothed and grid blasted substrate, with roughness \( R_0, R_1, R_2 \) and \( R_3 \), were assumed for modelling shown in Figure 5.15. Impact velocity of the copper powder was increased from 400 to 600 m/s while impact temperature was varied from 400 \( K \) to 600 \( K \). The temperature rise on particles and substrate is based on the empirical assumption that 90 % of plastic work under adiabatic conditions is dissipated as heat.
Figure 5.15: Randomly created substrate roughness profiles.

Wu et al. [75] explained that the adhesion energy is a function of contact area, contact temperature and contact time. In order to get a clear idea about the interface parameters such as contact time, contact temperature and contact area, numerical modelling results are discussed. Figure 5.16 shows the contact time and contact area for the particle impact on a smooth and roughened. In general, the contact area and contact area is not linear with the increment of roughness. Both the contact time and contact area are higher for $R_2$ and $R_3$ while a small decrease in contact area is observed for $R_1$ compared to smooth surface.

Figure 5.16: Effect of substrate roughness on particle impact time and contact area
The bonding mechanism can be influenced by factors such as velocity and initial temperature of particles, etc. Figure 5.17 shows the comparison of contact area of particle impacts on smooth and roughened substrates for different impact velocities. It is clear that increasing impact velocity increases the contact area values. Figure 5.18 shows the comparison of contact area of particle impact for different impact temperature with identical impact velocity. It is shown that the contact area will slightly increased by 1% with the increment of initial temperature.

Figure 5.17: Effect of particle impact velocity on contact area

![Impact Temperature 500K](image)

Impact Temperature 500K

Contact Area (m²) x 10^-9

Impact Velocity (m/s)

Figure 5.18: Effect of particle impact temperature on contact area

![Impact Velocity 500m/s](image)

Impact Velocity 500m/s

Contact Area (m²) x 10^-9

Impact Temperature (K)

Figure 5.19 shows the deformed pattern of the copper particles on different aluminium substrates at same impact velocity and the corresponding interface temperature values. From the simulation data, it is clear that increasing substrate roughness increases the interface temperature.

Figure 5.19: Deformed pattern of copper particles on different aluminium substrates

Figure 5.19 shows the deformed pattern of the copper particles on different aluminium substrates at same impact velocity and the corresponding interface temperature values. From the simulation data, it is clear that increasing substrate roughness increases the interface temperature.
The interface temperature for roughened substrates at contact time are higher than that of smooth case. And among roughened substrates, the interface temperature for $R3$ is higher among all the cases. Among the roughness cases, from the interfaces of the deformed particles, it is clear that the maximum interface temperature distributions for smooth and highly roughened substrate are localized in a small region. However, in roughness case $R3$, where roughness value is $1/7$ to that of particle size, the maximum temperature distribution is extended to the particle’s interior rather than along the interface between particle and substrate contact region.

![Figure 5.19: Effect of substrate roughness on temperature rise. Particle impact velocity 600m/s and particle impact temperature 500 K](image)

### 5.4 Discussion and Conclusion

A fully molten and a semi-molten YSZ droplet were simulated to impact onto a solid stainless steel substrate. A $30 \mu m$ fully molten ceramic powder with a impact velocity of $190 \ m/s$ was created as a benchmark. The morphology, flattening degree during the whole process was examined. The final splat trend showed a good likeness to an experimental and analytical comparison. With the increase of the initial velocity, the flattening degree will increase as well. Also, elevating the impact velocity will introduce plastic deformation on the stainless steel substrate. The higher the velocity is, the larger the plastic strain will be. Moreover, with the contact of the two parts, the temperature of the contact part on the liquid will decrease, thus the viscosity will increase and stop the flow locally, finish the solidification, form a thick part in the centre of the splat.

A $80 \mu m$ semi-molten particle with different solid core size impingement simulation was then performed. The splat morphology during the whole process was obtained and also the deformation of the solid core was captured. The smaller the solid core is, the larger the flattening...
degree will be. Also, the normalized deformation factor is proportional to the size of the core.

A systematic study was then performed on semi-molten particle with solid shell and liquid core. The computational results show that with the identical liquid volume fraction, whatever the particle size is, there would be almost no change on the interested parameters. Increasing the velocity of the particle would result in a higher contact temperature for both particle and substrate. With the similar particle size, the larger the liquid core is, the larger the plastic deformation could be seen at the contact area. Dramatic increase of contact area could be seen for liquid core fraction larger than 50%.

At last, the effect of roughness of substrate’s surface was studied. Metallic material was utilized in order to have a direct impression on the plastic deformation. The results show, impacting particles get plastically deformed more severely locally on roughened substrate than the smooth cases to obtain higher temperature and strain values. The contact time, contact area and interface temperature are higher on the $R2$ and $R3$ substrates, while negative effect for $R1$ is observed due to contact area decrease. It is suggested that substrate roughness whose average asperity size is higher than the $1/10$ of particle size is beneficial, while average roughness much smaller than the $1/10$ of particle size may result in weaker adhesion than this of smooth surfaces. Bond strength values for grit-blasted substrates are higher than the smooth cases due to the enhanced mechanical interlocking through the increase in contact area and contact time which plays an important role in bonding mechanism.
Chapter 6

Numerical study of particle impingement by utilizing SPH method

6.1 Introduction

A CEL method was developed and validated in Chapter 5. Most semi-molten particles impingement could then be simulated by utilizing this numerical method. Not only the large deformation of the liquid but also the plastic/elastic deformation of solid part could be modelled. Local temperature increase due to the dissipation of plastic deformation could also be extracted. Therefore, this model is more accurate in case of semi-molten droplet impingement. In this experiment, most VA particles whose size is smaller than 25 $\mu m$ were well melted and the viscosity of the particle is relatively low ($< 1$ Pas). These particles would behave quite similar to a Newtonian liquid. However, some large particles would remain in glass-state or "soften" state. According to the literature [95–97], at the temperature around the melting point (around 1200 $^\circ$C) the viscosity of the particle would increase dramatically from $< 1$ Pas to around 100 Pas. According to the experiment record, these particles would behave like a viscoelastic material. Although conventional Finite Volume Method (FVM) shows its great potential in solving droplet impact problems [73–75, 77], the time-step is required to decrease rapidly with the increment of viscosities, in order to have a stable solution to Navier-Stokes equations. Conventional Volume of Fluid method (VOF) and Coupled Eulerian and Lagrangian (CEL) method were initially adopted to solve the high-viscosity particle impact case. Figure 6.1 and 6.2 illustrate the results. The former graph is the simulation of Laki VA particle impingement with initial velocity of 10 $m/s$ and with a viscosity of 1 $Pas$. A symmetric 2D model was built in FLUENT and VOF method was used. It took a DELL 7300 WORKSTATION around 4 days to
run the simulation. The latter graph shows the simulation results with same initial condition but with viscosity of 0.1 Pas. A symmetric 3D model which is identical to the fully-molten model in Chapter 5 was built and CEL method was used. The calculation took around 3 days to accomplish. The simulation would be very time-consuming and costly computationally if the viscosity and velocity are increased. For the reason mentioned above, a fast and accurate approach is required in order to perform the systematic study for high-viscosity VA particle impingement cases.

![Figure 6.1: Numerical results for Laki particle impingement with viscosity of 1 Pas by VOF method](image1)

![Figure 6.2: Numerical results for Laki particle impingement with viscosity of 0.1 Pas by CEL method](image2)

The Smoothed Particle Hydrodynamics (SPH) method seems to be a proper solution to this problem. SPH is a meshfree particle method based on Lagrangian formulation. It was first invented to solve astrophysical problems in three-dimensional open space [78, 79]. Unlike
conventional mesh based Eulerian Solver, in SPH, the state of a system is represented by a set of particles, with possess material properties and interact with each other within the range controlled by a weight function or a smoothing function. Figure 6.3 briefs the difference between FVM method such as VOF and meshless method such as SPH.

![Figure 6.3: Difference between FVM method and meshless method](image)

Many researchers have done works to improve or modify the original SPH method for various applications. For example, Gingold and Monaghan found the non-conservation of linear and angular momentum of the original SPH algorithm, and then introduced an SPH algorithm that conserves both linear and angular momentum [80]. Hu and Adams also invented an angular momentum conservative SPH algorithm for incompressible viscous flows [81]. The overview written by M. R. Liu and G. R. Liu [149] elaborates history and development of the SPH algorithm. In this chapter, original SPH algorithm was integrated with heat transfer function and implemented by C/C++ code. Systematic study was performed based on the numerical model. Numerical results were collected, examined and compared with experimental data.

### 6.2 Methods

The conventional SPH method was originally developed for hydrodynamics problems in which the governing equations are in strong form of partial differential equations of field variables such as density, velocity, energy, and etc. There are basically two steps in obtaining an SPH formulation. The SPH formulation was obtained by particle approximation. In this step, the computational domain is discretized by representing the domain with set of small particles.
These particles were initialized with initial settings of the problem. After the discretization, field variables on a particle are approximated by a summation of the values over the nearest neighbour particles. Figure 6.4 demonstrate the initial discretization of the computational domain. The viscous VA particles are discretized into red particles, while the substrate was discretized in blue particles.

Figure 6.4: Initial discretization of the computational domain
6.2.1 SPH Approximation Techniques

The field variables (density, velocity, energy etc.) on this set of particles was then estimated. Equation 6.1 is the discretized form of the continuous kernel approximation.

\[
< f(x) > = \sum_{j=1}^{N} \frac{m_j}{\rho_j} W(x_i - x_j, h)
\]  

(6.1)

where \(i\) is the particle of interest, \(W\) is the smoothing function that is used to approximate the field variables at particle \(i\) using averaged summations over particles \(j\) within the support domain with a cut-off distance of \(h\). \(N\) is the total number of particles within the influence. Figure 6.5 represents the SPH particle approximation in a two-dimensional problem domain.

![Figure 6.5: SPH particle approximations in a two-dimensional problem domain \(\Omega\) with a surface \(S\).](image)

This procedure of summation over the neighbouring particles is referred to as particle approximation, which states that the value of a function at a particle can be approximated by using the average of the values of the function at all the particles in the support domain weighted by the smoothing function. Following the same procedure, the particle approximation of a derivative can be obtained as in Equation 6.2

\[
< \nabla f(x) > = - \sum_{j=1}^{N} \frac{m_j}{\rho_j} f(x_j) \nabla W(x - x_j, h)
\]

(6.2)

where the gradient \(\nabla W\) is evaluated at particle \(j\). This equation shows the approach of evaluating the gradient of the field variables at a particle located at \(x\). By implementing equation 6.1 and 6.2, the N-S equations in SPH equation of motion could be written as:

\[
\frac{D\rho_i}{Dt} = - \sum_{j=1}^{N} m_j v_{ij}^{\beta} \frac{\partial W_{ij}}{\partial x_i^{\beta}}
\]

(6.3)
\[
\frac{Dv_i^\alpha}{Dt} = -\sum_{j=1}^{N} m_j \left( \frac{\delta_j^{\alpha\beta}}{\rho_j^2} + \frac{\delta_j^{\beta\gamma}}{\rho_j^2} \right) \frac{\partial W_{ij}}{\partial x_i^\beta} + F_i \quad (6.4)
\]

\[
\frac{De_i}{Dt} = -\frac{1}{2} \sum_{j=1}^{N} m_j \left( \frac{p_i}{\rho_j^2} + \frac{p_j}{\rho_j^2} \right) v_{ij} \frac{\partial W_{ij}}{\partial x_i^\beta} \quad (6.5)
\]

where \( v_{ij} = v_i - v_j \). These set of equations are the commonly used SPH equations for the N-S equations. However, by using different numerical tricks, it is possible to get other forms of SPH equations for these partial differential equations. For example, in this study, in order to simplify the calculation, the field function of density was estimated by the following equation proposed by [150].

\[
\rho_i = \sum_{j=1}^{N} m_j W_{ij} \quad (6.6)
\]

### 6.2.2 Selection of SPH Smoothing Function

One of the central issues for meshfree methods is how to effectively perform function approximation based on a set of nodes scattered in an arbitrary manner without using a predefined mesh or grid that provides the connectivity of the nodes [149]. In the SPH method, due to the fact that the smoothing function is used for kernel and particle approximations, it is very important to choose the most suitable one. Smoothing function has been studied mathematically by different researchers in order to improve the performance. Lucy [78] in his original paper proposed a bell-shaped function. Monaghan and Lattanzio [82] has proposed a Cubic B-Spline smoothing function which is the most frequently used ones.

\[
W(R, h) = \alpha_d \left\{ \begin{array}{ll}
\frac{2}{3} - R^2 + \frac{1}{2} R^3 & 0 < R < 1 \\
\frac{1}{6}(2 - R)^3 & 1 \leq R < 2 \\
0 & R \geq 2
\end{array} \right. \quad (6.7)
\]

where \( R = r/h \), \( r \) is the distance between particle i and j, \( h \) is the domain cut-off distance. In three-dimensional space, \( \alpha_d = \frac{32\pi}{3} h^3 \). This smoothing function is widely used since it closely resembles a Gaussian function while having a narrower compact support.

Higher order splines (quartic and quintic spline) was introduced by Morris [83, 84]. Johnson et al. [85] used the following quadratic smoothing function to simulate high velocity impact problems.

\[
W(R, h) = \alpha_d \left( \frac{3}{16} R^2 - \frac{3}{4} R + \frac{3}{4} \right), \quad 0 \leq R \leq 2 \quad (6.8)
\]

where in three-dimensional space, \( \alpha_d = \frac{5}{4\pi} h^3 \). The derivative of this quadratic smoothing function always increases as the particles move closer, and always decrease as they move apart. In this case, the movement of the particles would be more stable undertaking large compressive force during impact.
6.2.3 Implement of Heat Transfer and Solidification

Following the method of SPH algorithm, the heat transfer function was then discretized from differential equation 6.9 to the SPH equation 6.10.

\[
\frac{dT}{dt} = \alpha \nabla^2 T \quad \text{(6.9)}
\]

\[
\left( \frac{dT}{dt} \right)_i = \alpha \frac{1}{2} \left( \sum_j x_{ij} \frac{m_j}{\rho_j} W + \sum_j y_{ij} \frac{m_j}{\rho_j} W + \sum_j z_{ij} \frac{m_j}{\rho_j} W \right)
\]

\[
= \frac{2}{\rho_i} \sum_j \frac{m_j}{\rho_j} (T_j - T_i) W \quad \text{(6.10)}
\]

By using the equations above, temperature of every single particle could be calculated. The solidification process is simulated by manually eliminating the velocity to all directions to zero for particles whose temperature is lower than the melting point. In this way, the temperature of the particle which is close to the substrate would drop quickly. The closer the distance is, the faster the temperature would drop. Particles with local temperature lower than the melting point was stagnated. Solidification of the contact area would be simulated.

The SPH algorithm mentioned equations mentioned above was then implemented by C++ code. A 2D case was initially generated, the results was displayed by utilizing OpenCV library. The simulation was then improved to 3D cases and numerical results were visualized by using MATLAB. Comparing with VOF and CEL method mentioned at the beginning of this chapter, with the identical computational resources, the simulation time was shortened by around \( \frac{3}{4} \). A systematic study was then performed by using this SPH model. The viscosity, angle of incidence (contact angle) were examined. A 20 \( \mu m \) VA particles was created as a benchmark. Viscosity of the viscous droplet was varied from 1 Pas to 50 Pas. The angle of incidence was tested at 30, 60 and 90° (normal impact) respectively.
6.3 Results

6.3.1 Property of Materials

In order to build numerical models to simulate the VA particles impingement, the thermo-properties of VAs are essential. However, due to the small size of VA particles, most properties could not be measured directly. Kucuk et al. [95], Giordano et al. [96] and Fluegel et al. [97] have related the density, viscosity and surface tension with VA chemical composition and temperature. Based on the equations mentioned in [95–97], the temperature and composition dependent density, viscosity and surface tension of all four types of VAs are calculated and shown Figure 6.6. The surface tension of Laki, Hekla, Askja and Eldgja at 1400°C are 388, 329, 320 and 391 mN/m respectively.

![Figure 6.6: Temperature and composition dependent viscosity and density of four types of volcanic ash](image)

6.3.2 Numerical Study of 3D Viscous CMAS Impingement with Solidification

Figure 6.7 illustrates the whole impingement process and solidification by using SPH method. The viscous droplet hits the substrate with 90°. The droplet starts to deform initially. The bottom part would start to solidify prior to the top part of the droplet. Furthermore, the deposition would start to solidify from the bottom to the top. Most of the kinetic energy would dissipated by the viscosity. And finally after a certain time, the temperature of the droplet deposition would have the same temperature as that of the substrate.
Figure 6.7: Heat transfer for droplet with viscosity of 0.1 Pas and velocity of 10 m/s. Unit of the all axis is µm. a) 0.5 µs after impact, b) 1.5 µs after impact, c) 3 µs after impact d) 10 µs after impact
Figure 6.8 depicted the final deposition of particles with different viscosities. It is very clear that the larger the viscosity is, the smaller the spreading factor would be. The spreading factor would decreased from 1.23 to 1.01 with the increase of the viscosity.

(a)

(b)

(c)

Figure 6.8: Final deposition of droplet with viscosity of (a) 1 Pas (b) 10 Pas and (c) 50 Pas for normal impact. Unit of the all axis is $\mu m$. 
Figure 6.9 illustrate a representative oblique impingement process. The viscous droplet was initialized with the same velocity magnitude but also with a angle of incidence. Therefore, the droplet would travel not only vertically but also horizontally. As long as the droplet get near the substrate, the bottom part of the droplet would start to solidify. At the same time, the top part of the drop let would continue moving in the horizontal direction. Therefore, the spreading factor for the oblique impact is much larger than the normal impact. For this specific case shown in Figure 6.9d, the spreading factor was 1.98 compared with only 1.01 for normal impact.
Figure 6.9: Impingement process for droplet with viscosity of 50 and 30° angle of incidence. Unit of all axes is µm. a) 1 µs after impact, b) 2 µs after impact, c) 3 µs after impact d) 5 µs after impact
Another interesting phenomena could be seen in Figure 6.10. For droplet with lower viscosity in oblique impingement case, temperature of the bottom part of the substrate would solidify while only little kinetic energy would dissipated by the viscosity term. The particle would start to bounce back. At the time the kinetic energy for bouncing back is higher then the internal force between particles, break up was seen. The bottom part of the particle would stick on the substrate while the top part of the particle would bounce away. The splat morphology of small particles (Figure 6.11) proves the phenomena observed in the numerical model. In the numerical result, a clear break up could be seen after the oblique impact due to solidification at the bottom of the particle and the surface tension is not enough to hold the droplet. At the edge of the droplet deposition in SEM in Figure 6.11 micrograph, clear imprint of droplet oblique impingement and breakup could be seen.

![Figure 6.10: Final deposition of droplet with viscosity of 1 Pas and contact angle of 30°](image)

![Figure 6.11: SEM micrographs of deposition of 25 μm Laki particle impingement](image)

Figure 6.12 compares the results from the numerical model with the SEM collected from the experiment. As has been discussed in Chapter 4, medium particles would only be softened and would have relatively high viscosity. In this case, the kinetic energy would dissipate more by the viscosity. The whole droplet would remain a round shape and would not break up. The evidence
of oblique impact could also be seen in this splat morphology. In the sub-figure at bottom left of Figure 6.12, the right edge of the particle is thinner while the left edge is thicker. The similar results could be seen in high viscosity droplet impingement with high contact angle. It could be assumed that, in the experiment, the droplet impacted on the substrate with also a horizontal velocity. In this way, the top part of the viscous droplet would continue moving to the left while the bottom part solidified on the right. A thin to think splat morphology was then formed.

Figure 6.12: Comparison between SEM micrograph of medium size Laki droplet with relatively high viscosity and the numerical model

6.4 Discussion and Conclusion

In this chapter, SPH algorithm was introduced to calculate the motion of high-viscosity particle impingement. This Lagrangian based method is less time consuming in simulating the high viscosity particle impact. The viscous droplet were treat as a combination of finite small particles and Navier-stokes equations were than discretized into a summation form. Suitable smoothing function were selected to perform the simulation. Apart from the N-S equations, heat transfer equation were also discretized in the SPH form. Therefore, the solidification as well as the heat transfer between the substrate and particles itself could be simulated. A systematic study was then performed by utilizing this numerical model. The effect of impact angle, viscosity were examined. The results show that the contact angle would play a very important role in the spreading factor. The higher the contact angle is, the larger the spreading factor would be. The
spreading factor would increase from 1.01 to 1.98 along with the increment of contact angle from 90 degree (normal impact) to 30 degree. Moreover, the particles wish lower viscosity and high contact angle would result in a break up. This phenomena could be validated by the SEM micrograph from the experiment. Small particles tend to have lower viscosity and high contact angle. An obvious break up could be seen in the micrograph of the deposition.
Chapter 7

Conclusion

7.1 Thesis Summary

The objective of this thesis was to understand the details of sticking and bonding mechanism of VA particles and the substrate by utilizing numerical models. In particular, experiments (Chapter 3) were performed by Dr. James Dean and Dr. Catalina Taltvull to reproduce the environment of a combustion chamber in jet engine. Different types of volcanic ash were introduced into the VPS and delivered towards the substrate, in order to simulate the scenario of VA impingement onto turbine blades. The composition and properties of VAs were measured and the experimental data, including temperature and velocity of the flow field, splat morphology of the VA deposition and adhesion rate of the VAs, were collected. Numerical model was built by the author to study the details of the heat transfer and non-isothermal effect of in-flight particles (Chapter 4), the deformation, morphology, heat transfer and phase transition of semi-molten particle impingement (Chapter 5), the morphology and solidification of glass-state (high viscosity) particle impingement (Chapter 6). Ultimately, the findings presented in this thesis advance the fundamental understanding of particle impingement and bonding mechanism. Moreover, the thesis offers a research approach to perform a study of simulating high-speed, high temperature particle impingement.

Primary conclusions can be drawn as a summary of the results presented in the preceding chapters. First, the findings presented throughout the first numerical model clearly demonstrate the coupled effect of grain size of and non-isothermal effect within VA particles. The result shows for small particles, although it would be easily melted, it would be also simply carried by the flow and bypass the substrate or hit the substrate with a large contact angle. On the contrast,
large particles would not be easily influenced by the carrier jet flow, and would more likely to perform a normal impact onto the substrate. However, due to the short travel time and large grain size of these particles, these particulate would remain unmelted during impact. Unmelted particles are more likely to result in plastic damage on the substrate but less likely to adhere to the substrate and cause more severe damage. The particles size from $15 \mu m$ to $40 \mu m$ were characterized, by this numerical model, as the most dangerous particles for the reasons that they have both high adhesion rate as well as high possibility of hitting the substrate.

Second, a systematic study of semi-molten particle impingement were performed by utilizing the CEL model developed by the author. By utilizing this model, the solid part would no longer be treated as rigid body. In this way, a more accurate deposition morphology of semi-molten particle impingement could be simulated. The influence of impact velocity, volume fraction of liquid part, size of the particle, roughness of the substrate were studied by using this numerical model. The contact area, contact time, heat transfer and phase transition were collected and studied. The results shows that for particles whose liquid volume of fraction is greater than 50 %, the particle would soften to a large extend, thus cause large deformation and large contact area. For the particles with higher initial kinetic energy, large plastic deformation could be seen on both substrate and particles. And there would be more heat generated by the dissipation of kinetic energy. The local maximum contact temperature is higher for particles with higher impact velocity. And the study of the roughness shows, substrate roughness whose average asperity size is higher than the $1/10$ of particle size is beneficial, while average roughness much smaller than the $1/10$ of particle size may result in weaker adhesion than this of smooth surfaces. Bond strength values for grit-blasted substrates are higher than the smooth cases due to the enhanced mechanical interlocking through the increase in contact area and contact time which plays an important role in bonding mechanism.

Third, SPH algorithm was introduced to calculate the motion of high-viscosity particle impingement. This Lagrangian based method is less time consuming in simulating the high viscosity particle impact. The viscous droplet were treat as a combination of finite small particles and Navier-Stokes equations were then discretized into a summation form. Suitable smoothing function were selected to perform the simulation. Apart from the N-S equations, heat transfer equation were also discretized in the SPH form. Therefore, the solidification as well as the heat transfer between the substrate and particles itself could be simulated. A systematic study was then performed by utilizing this numerical model. The effect of impact angle, viscosity were examined. The results show that the contact angle would play a very important role in the spreading factor. The higher the contact angle is, the larger the spreading factor would be. The spreading factor would increase from 1.01 to 1.98 along with the increment of contact angle from 90 degree (normal impact) to 30 degree. Moreover, the particles with lower viscosity and high contact angle would result in a break up. This phenomena could be validated by the SEM
micrograph from the experiment. Small particles tend to have lower viscosity and high contact angle. An obvious break up could be seen in the micrograph of the deposition.

7.2 Future Directions

Although the experiment is tend to completely simulate the environment of combustion chamber and turbine section, there still remains some questions. The key concern of this set up would be the chamber pressure. The pressure for the VPS system is from 80 mbar to 120 mbar which is 1/10 to 1/100 of that in a realistic jet engine. Firstly, the VPS system is, to the best of the knowledge of all researchers in this group, the most suitable apparatus to generate a high temperature and high velocity field. Meanwhile, the temperature and velocity could be easily measured by using the VPS system. Furthermore, the VPS is designed to deliver coating powder towards the base material. Therefore, minimum modification is needed in order to deliver VA powder towards the substrate. Secondly, the aim of this study is to understand the correlation between different interested parameters and the sticking rate/bonding mechanism of volcanic ash. Pressure is not known to have significant effect on the sticking rate or bonding mechanism. Therefore, the further study would be focus on the field of pressure itself. Suitable experiment rig is required to examine the effect of pressure. Moreover, if there exists an experiment rig which can stand high pressure while can also generate high temperature and high velocity field, the approach in this thesis could be easily replicated in the new experiment set-up.

As with any research of this magnitude, each conclusion appears to be replaced with more questions. Fortunately, the approach established in this thesis could be utilized for any systematic study of similar particle impingement cases. The numerical model developed in this thesis are mainly concentrate on a micro scale. The bonding mechanism are largely related to the morphology/splat deposition of the particle as well as the heat transfer between the particle and the substrate. Further study could be done on molecular-scale. A molecular dynamic model (MD) would help understand the fundamental physics bonding or chemical reaction for the adhesion mechanism.

7.3 Final Remarks

Upon beginning this research, most research work related to the correlation of CMAS and TBC are focused on the area of coating damage after CMAS adhesion. Other works done on this field are on a macro-scale, statistics data are collected. However, there is no detailed study, especially in micro-scale, with the research focus on the impingement process. This thesis performed a systematic study on the fundamental understanding of VA particle impingement and bonding mechanism in micro-scale, and for the first time, the impingement of VA particles of
high velocity and high temperature coupled with non-isothermal effect and phase transition were studied. Numerical models are developed and validated by the experiment data. Influence of interested parameters are studied based on the numerical model. Splat morphology and bonding mechanism are analysed. The author hopes that the foundations established here will contribute to the understanding of the CMAS damage on the TBCs and will propagate to shed light on the abundance of unresolved questions in this field.
Bibliography


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Appendix A

Glossary and Results data

Please find the attached DVD-1 to see:

A2. The experiment data and SEM micrographs for test case A B and C
A3. The animation of particle impact by using SPH algorithm
A4. The project presentations by the author
Appendix B

Source Codes

Please find the attached DVD-2 to see:

B1. The UDF Code to calculate non-isothermal effect of ceramic particles

B2. C/C++ Code of SPH model, also 2D/3D model available on https://github.com/kpshadow