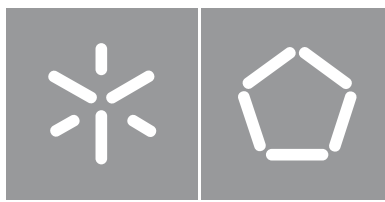


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Computational Modelling of the Selective Laser Sintering Process



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Computational Modelling of the Selective Laser Sintering Process

Master's Dissertation

Integrated Masters in Polymer Engineering

Work accomplished under the supervision of:

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To everyone, I am so grateful for your support, as I could have not done it without you.

Statement of integrity

I hereby declare having conducted this academic work with integrity. I confirm that I have not used plagiarism or any form of undue use of information or falsification of results along the process leading to its elaboration. I further declare that I have fully acknowledged the Code of Ethical Conduct of the University of Minho.

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Resumo

A Manufatura Aditiva (AM do inglês *Additive Manufacturing*) tem ganho popularidade em várias indústrias importantes e exigentes devido à sua capacidade de produzir peças com geometrias complexas e pouco desperdício. Como uma das suas mais populares técnicas, a Sinterização Seletiva a Laser (SLS do inglês *Selective Laser Sintering*) é muito procurada por diversas indústrias que pretendem substituir processos convencionais mais dispendiosos. No entanto, o processo de SLS é intrinsecamente complexo devido aos vários fenómenos multi-físicos e são necessários mais estudos para obter uma melhor perceção dos mesmos. Isto tem originado um elevado interesse académico em otimizar o processo para que este cumpra os requisitos industriais. Grande parte destas otimizações são feitas através de métodos experimentais que são demorados, dispendiosos e nem sempre resultam nas configurações ótimas. Este enquadramento tem motivado investigadores a recorrer à modelação computacional com o objetivo de entender melhor o processo, de modo a antecipar e corrigir defeitos.

O objetivo principal do presente trabalho foi desenvolver um modelo capaz de simular o processo de SLS para aplicações poliméricas, em código de distribuição livre, à escala do tamanho da partícula. Como são necessárias abordagens distintas para simular com precisão cada etapa do processo, diferentes métodos numéricos foram aplicados para desenvolver uma ferramenta capaz de estudar o impacto, numa secção representativa da cama de pó, dos parâmetros físicos que podem ser ajustados no processo.

O trabalho desenvolvido integrou diversas etapas, começando por um estudo extenso dos aspetos teóricos do processo de SLS que visou a familiarização com os fenómenos envolvidos, o desenrolar do processo, os seus parâmetros e respetivas influências, assim como a avaliação das limitações e desafios existentes. Este estudo foi seguido por uma análise detalhada dos modelos mais populares empregues para representar os principais fenómenos associados ao processo e do nível de precisão das abordagens, com base nas simplificações consideradas. Um conjunto de ferramentas computacionais foi posteriormente apresentado e os seus respetivos modelos selecionados, quando possível, de acordo com a revisão bibliográfica efetuada. Por último, vários testes foram executados, visando uma validação experimental qualitativa dos códigos utilizados, para garantir que o modelo em uso era adequado para simular o processo, permitindo o estudo e observação da influência dos principais parâmetros do processo e a evolução da sinterização.

Os desenvolvimentos obtidos representam um avanço significativo para a simulação do processo de SLS. Com o uso de *software open-source* (LIGGGHTS e OpenFOAM), vários estudos foram feitos numa geometria realista e, apesar da ausência de dados experimentais suficientes e mais detalhados, os resultados da simulação mostraram-se bem correlacionados com os usados para comparação. Em suma, o trabalho efetuado permitiu concluir que a ferramenta desenvolvida apresenta um elevado potencial para estudar, com detalhe, o processo de SLS e a influência dos seus parâmetros e, deste modo, contribuir para a sua otimização.

Palavras-chave: Sinterização Seletiva a Laser (SLS), polímeros, modelação numérica, OpenFOAM, LIGGGHTS

Abstract

Additive Manufacturing (AM) has increased in popularity in numerous important and demanding industries due to the capability of manufacturing parts with complex geometries with little wastage. As one of its most popular techniques, Selective Laser Sintering (SLS) is sought after by several industries that aim to replace conventional and more expensive processes. However, the SLS process is intrinsically complex due to the various underlying multi-physics phenomena and more studies are needed to obtain more insights about it. These has resulted in many academical interests to optimize the process and allow it to achieve industrial standards. Most of these optimization attempts are performed through experimental methods that are time consuming, expensive and do not always provide the optimal configurations. This has lead researchers to resort to computational modelling, aiming at better understanding the process to anticipate and fix the defects.

The main objective of the present work was to develop a model capable of simulating the SLS process for polymeric applications, within an open-source framework, at particle length scale. Since distinct approaches are required for accurately simulating each step of the SLS process, different numerical methods were employed to develop a tool capable of studying the impact, in a representative section of the powder bed, of the physical parameters that can be adjusted in the process.

The developed work comprised several steps, starting with an extensive study of the theoretical aspects of the SLS process that aimed at the acquaintance with the involved phenomena, process unwind, its parameters and their influence, as well as evaluating the existing limitations and challenges. This study was then followed by a detailed analysis of the most common employed models to represent the major phenomena and of the accuracy level of the approaches, based on the employed simplifications. A set of computational tools was then exhibited and their built in models were selected, when possible, according to the precedent literature review. Lastly, various tests were carried to obtain an experimental qualitative validation of the used code, to assure that the used model was adequate to simulate the process, allowing the study and observation of the principal parameter influence and sintering progression.

The achieved developments represent a significant advance towards the SLS process simulation. With the use of open-source software (LIGGGHTS e OpenFOAM), several studies were performed on a realistic geometry and, despite the absence of enough and more detailed experimental data, the simulation results are in agreement with the ones used for comparison. Overall, the accomplished work allowed to conclude that the developed tool constitutes a great potential to study, in detail, the SLS process and its parameters influence and, therefore, contribute to its optimization.

Keywords: Selective Laser Sintering (SLS), polymer, numerical modelling, OpenFOAM, LIGGGHTS

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CHAPTER 1 Introduction

1.1 Additive Manufacturing

Additive Manufacturing (AM) is the formal designation for Rapid Prototyping and is commonly referred to as three-dimensional (3D) printing. AM is the opposite of subtractive manufacturing, where the initial shape of the part is a block, bar or rod, from where material is removed through various operations, such as cutting, boring, drilling and grinding, that can be done manually or, more commonly, automatically, with the use of Computer Numerical Control (CNC), as seen in the manufacturing of moulds employed in plastic injection moulding. AM is not a single process, but a set of technologies grouped together that share the characteristic of building parts layer-by-layer, which allows for more complex geometries and the production of objects with virtually any shape. Building in such a way removes the need of extra tooling and reduces material waste, since the only material used is the one present in the final part (with the exception of support structures). Also, the unneeded external tools or moulds makes AM processes a cheaper, faster and, therefore, viable option for the production of parts in small quantities and prototypes, especially when considering how easy it is to iterate the design.

Layer-by-layer printing was used as early as the 19th century in areas such as topography and photosculpture [1] with simpler materials, such as cardboard and wax. These uses inspired the development of processes that would later result in modern AM techniques. For example, in 1951, Munz [2] disclosed a system, with features of nowadays stereolithography, for selectively exposing a transparent photo emulsion in layers, where each of them comes from a cross section of a scanned object. In 1968, the first process of a three dimensional polymerization with lasers was proposed by Swainson [3], but it never achieved a viable commercial process. In 1971, Ciraud [4], proposed a powder process with all the features of modern direct deposition and, in 1979, Housholder [5] presented, in a patent, the earliest description of a powder laser sintering with detailed information on the layer deposition and selective scanning. Subsequently, in the late 1980s, similar and more refined

processes were developed, aiming for the commercial use of AM that was achieved in the 1990s, and, since then, its popularity has been growing exponentially [6, 7]. Nowadays, AM is being applied in a wide range of relevant technological fields, such as biotechnology, aerospace, robotics, environment, energy, automotive and common industry [6].

The AM process comprises three main stages [8]:

1. The first step is the digital modelling of the part in a Computer Aided Design (CAD) software and its conversion to a compatible format, generally the Standard Tessellation Language (STL), so it can be sent to the AM machine.
2. Next, the modelled geometry is manipulated by the machine to assure that it is oriented, positioned and sized correctly, as well as virtually sliced by horizontal parallel cuts, with a specified thickness, that represent the layers and work as guides for the printing stage.
3. Lastly, the building process, which occurs mostly automatically, often just requiring superficial monitoring to avoid the occurrence of errors. When it ends, the part is safely removed and optional post-processing steps, such as removal of supports, dusting and sanding, are performed.

The printing and characteristics of a part vary significantly depending on what technology and process parameters are used for its manufacture. Different methods have distinct layer bonding strategies and ways to split and support them, meaning that equal, or very similar, geometries, result in dissimilar parts when different technologies, or machines within the same technology, are being used. There are a variety of options when it comes to selecting a process due to the large number of technologies based in AM. The same applies to materials, with polymers being the most popular due to their processability, low cost and unique properties [9, 10]. All of these approaches, paired with the different materials used, will determine factors such as the printing speed, mechanical properties and accuracy of the final product [8].

1.2 Powder Bed Fusion

According to the ASTM technical committee [11], Powder Bed Fusion (PBF) is one of the seven main AM processes. It was one of the earliest developed and commercialized techniques and, up until today, this methodology remains one of the most versatile due to various possible energy sources, machine configurations, materials, such as polymers, metals and, less commonly, composites and

ceramics [12], and ways to bind them together. The PBF process, as the name suggests, consists in the fusion of a powdered material that is located in the machine bed. It can be divided into three main steps: (i) powder recoating, where a new layer of material is spread evenly, (ii) energy input, which involves transfer of thermal energy from a heat source to the material and, lastly, (iii) material coalescence and cooling, where granules fuse and subsequently cool to a solid state. This process distinguishes itself from others within AM due to the use of high density energy sources, such as lasers and electron beams, being the former far more common. The use of lasers within the PBF process is known as Laser Sintering (LS) and, depending on the main fusion mechanism, technologies employed and patent related problems, various names are given to this PBF variant. One of those is Selective Laser Sintering (SLS), a patented name given to LS that has been widely used by almost everyone in the field, being frequently found in articles replacing the term LS.

The SLS process, being an AM technology, shares its already mentioned benefits. Besides those, it gained extra popularity due to the ability to integrate the technology into small scale machines that are cheaper and more practical than the industrial scaled counterpart [13]. Also, it is a process that does not require support structures, since the non melted particles act as integrated supports, which reduces material waste and allows for more complex designs. These particles can also be reused on different builds, a very attractive feature for economical and environmental reasons. This feature also facilitates the building of multiple parts in the same bed because the space required for supports is now free, thus increasing process efficiency. When compared to other popular AM processes, such as Fusion Deposition Modelling (FDM), SLS offers much higher resolution, accuracy and surface finish quality, mainly because of the laser spot and particles small size [14]. Despite not being the process with better results in these parameters, SLS is still the most popular amongst engineering applications because of the resulting parts mechanical properties and much faster printing speeds [14]. All these advantages led to SLS being increasingly used in important and demanding industries, such as automotive [15], aerospace [16] and biomedical [17].

Despite being easy to understand the basics of the different processes associated with SLS, it has been found that, when compared to other techniques, they are not as simple, accurate or reproducible as they may look, especially for thermoplastic parts [18]. That is because LS processes are intrinsically complex due to the various underlying multi-physics phenomena, therefore, more efforts are needed to obtain more insights about the process. Some of the main known limitations are associated with the shortage of compatible or appropriate materials and the fact that in order to work with these technologies, one must have knowledge and skills in multiple fields. Furthermore, there are still a

significant amount of process deficiencies that have not been fully eliminated due to its complexity, such as pores and microcracks [19], curling [20] (the combination of both shrinkage and warping) and distortion caused by residual stresses [21]. Most of these defects are a direct outcome of the accentuated temperature gradients induced during the heating and cooling cycles and, considering the amount of publications on the topic, significant efforts were put into solving them. Fixing problems via trial-and-error experimental method takes a vast amount of time, is expensive, unable to provide detailed information on the temperature profiles or stress fields and does not always provide the optimal configurations. For these reasons, researchers have been resorting to computational modelling, aiming at better understanding the process to anticipate and fix the defects without manufacturing physical prototypes.

1.3 Numerical Modelling and Simulation State-of-the-Art

Although it is possible to build a part using LS technology without simulating the process beforehand, that does not mean that it is not necessary or recommended. When building simple prototypes, the mechanical properties or visual appearance might not play a relevant role, however, when manufacturing parts with higher requirements, those tend to be very important. Accordingly, simulating the process beforehand is useful to predict errors and provide technicians with important insights to better understand the process, which might lead to optimizations on part design and process parameters. The determination of the temperature profiles in space and time is one of the most useful insights that the simulation of the process can provide and is, otherwise, challenging or even impossible to measure experimentally. With a simple thermal model, based on estimated heating and cooling rates, the temperature gradient of the material can be easily obtained over time, which, by considering a melting point, allows the measuring of the fusion depth (known as melt pool for metals) [22]. Although useful, such approach is often too simple and insufficient, thus the integration of fluid flow into the model is often necessary to obtain more useful information. Metals in their liquid state, for example, are very sensitive to density and temperature changes. Using the appropriate models, the velocity fields, that represent the molten flow, can be depicted [23]. Depending on the selected method, some phenomena may be implemented while others may not, as it will be further discussed.

There are different approaches for numerical simulations, which can be classified into two major groups: mesh-free and mesh-based, with the last being much more popular. Mesh-free alternatives are based on Discrete Element Method (DEM), Lattice Boltzmann Method (LBM), Optimal Transportation

Method (OTM) and Smoothed Particle Hydrodynamics (SPH), while mesh-based counterparts comprise the Finite Element Method (FEM), the Finite Difference Method (FDM) and the Finite Volume Method (FVM). The DEM is the most common mesh-free method employed for simulating the process, but mainly for the powder bed distribution [24]. It accounts for the discrete nature of the powder bed and considers the interactions between each particle at their contact point, being well suited for the study of granular media. Despite its elementary Newtonian mechanics, it has been extended to include other interactions between particles, such as heat transfer [25], that allowed the temperature distribution study within a realistic powder bed [26]. Unfortunately, this approach fails to consider the surrounding air or the fusion and coalescence of the particles. On the other end, mesh-based methods, such as the FEM, firstly introduced in 1956 [27], stands out for its extensive use for simulating the SLS process [28–30] due to its simplicity, efficiency and mainly the vast amount of literature on the subject over the past decades. Even though it provides useful information, such as the temperature evolution, liquid fraction and residual stresses, this method makes it difficult to account for volume shrinkage, layer deposition and the particle nature of the bed [31], which motivates some authors to opt for the FVM [32]. Also, since meshed-based methods turn out to be more cumbersome to simulate the powder distribution and deposition, DEM is often coupled with those approaches to take care of this step [33].

Unlike conventional manufacturing processes, such as injection and extrusion, whose process have been extensively studied and optimized in the past, the optimization of the SLS process is more recent. It is usually performed through experimental methods [34], but such approaches are time-consuming and expensive. The primary purpose of most simulations on the SLS process is to assess the influence of the various process parameters into the final part mechanical and geometrical quality. Although the process being the same, distinct modelling approaches are taken for different materials, mainly polymers and metals, due to their different behaviours. For example, metals are exposed to a much wider temperature range, so considering their temperature dependent properties is imperative [35]. Also, due to their reduced viscosity, liquid metal flows are heavily influenced by density variations and many other effects that need to be accurately modelled [36]. The numerical modelling of temperature distribution, deformation and thermal stresses of a SLS process is similar to that of multi-pass welding [37], which is an older technology that has been developed and modelled for more than four decades. Unfortunately, for the SLS process, the model has to be more advanced due to all the additional complex physical phenomena involved, such as the laser interactions with the powder, namely absorption, reflection and scattering. Despite being a relatively new technology, a significant amount of attempts to simulate the process was already done. Some approaches aimed at developing

a model and validating it by comparing simulation results with experimental ones [38], while others aimed at optimizing a process or study the influence of certain parameters. Considering the powder bed as a continuous media, Childs et al. [39] investigated the influence of laser power and scanning speed and Dai and Shaw [40] the influence of scanning pattern and speed on the temperature and stress fields. Bugeda et al. [41] also developed a model to simulate the 3D sintering process of a single track, obtaining data such as the temperature field, solid fraction and sintering depth. Similarly, Dong et al. [42] modelled the transient heat transfer during the sintering process while considering the phase transition, but also the temperature dependent material properties to evaluate the temperature and density distribution. A more accurate model, considering a more realistic volumetric heat source, was developed by Riedlbauer et al. [43] to predict melt pool dimensions and validate the results with experimental data. Still related to melt pool, Peyre et al. [44] and Foroozmehr et al. [45] tested the effects of the process parameters on its temperature distribution and dimensions, validating the results with experimental tests. Bierwisch et al. [46] developed a 2D model with a realistic powder bed for two different materials, where the various phases of the process, namely scan, heat dissipation and cooling, were considered. Osmanlic et al. [47] developed a similar model with an accurate laser source, where phenomena such as reflection, refraction and attenuation were considered, but for much shorter time scales and with the objective of assessing the bed density influence on the process. Some authors compiled and reviewed several studies [36, 48–51] and the interested reader is addressed to those publications. Besides isolated models, there are also some commercial softwares that offer the option to simulate the LS process, such as ANSYS [52], SIMULIA [53], COMSOL [54] and NETFABB [55]. Also, for DEM simulations, LIGGGHTS [56] and LAMMPS [57] are commonly used.

Modelling SLS processes comes with several challenges. There are non-linearities to be considered, such as the temperature dependence of the material properties. Besides that, the problem must be discretized both spatially and temporally and, depending on the model scale, very small time scales and high mesh resolutions might be needed, which requires a significant amount of computational power. For the interaction of the laser with the material, there are several different physical behaviours to consider, such as absorption, reflection and radiation, along with the subsequent heat transfer, phase transformation, moving interface between the different phases, fluid flow and possible chemical reactions. Moreover, the powder distribution also affects most of the previously mentioned aspects, so an adequate geometry definition is also needed. In the end, for an accurate AM simulation, one must model the addition of the material, have a realistic model for the heat source, account for the thermal losses, consider the temperature dependence of some properties, model

elasto-plastic stresses and strains, couple the thermo-mechanical behaviour in a manageable way and, finally, model phenomena that change material properties [58]. However, these requirements are computationally demanding, therefore it is important to verify if simpler models are also able to provide useful insights about the process. Because of all the complexity associated, one aims to start with a simple approach, while maintaining the main features taking place.

1.4 Motivation and Objectives

Since their arrival, AM technologies have shown an immense potential to fabricate parts in a way that, if the quality is achieved, would make conventional and other recent alternative methods look outdated. They proved to have the ability to improve everyone's life and be worth their attention, something that can be seen by the multiple industrial applications and the consequent exponential market growth [7]. With PBF being one of the most popular AM methods, SLS falls no short in potential when compared to the other AM processes. Indeed, the ability to easily manufacture parts with very complex geometries that would be impossible, or extremely hard, to achieve with other methods and would take multiple other technologies and waste a lot more energy and material, is the most prominent advantage of the SLS process and the main reason for its increasing attention in the industry. For these reasons, increasing efforts have been put into further improving the SLS process.

Despite the ever-increasing interest of the industry in the SLS process, this recent technology is still not fully dominated and the current limitations are still substantial, attending to the demanding and specific thermo-mechanical and visual characteristics of the parts required for several applications. In that regard, the numerical simulation turns out to be a very useful approach for a better understanding of the process, since one can observe and analyse details that would otherwise not be accessible with the conventional experimental approaches. Moreover, with a good understanding of the process and its parameters, the numerical simulation allows to acquire useful insight on the process control, to prevent defects, and to guide process optimization, to improve specific desired properties. Nonetheless, such a task is challenging due to the complexity of predicting accurately the effects of the process parameters changes, motivated by the process' complex nature.

The common practice to perform numerical studies of AM processes is to acquire a software license, which is expensive. Even after that, it is nearly (or even totally) impossible to get access to the code and adapt it to specific needs, because they are proprietary. This framework results in the

financial impossibility to utilize the software by everyone but large companies, and the users cannot know if the modelling approach is rigorous enough or adequate for their specific needs. For these reasons, the use of open-source software, such as OpenFOAM [59], is gaining attention and becoming more widespread with growing communities of users and developers, where one can, free of any cost, use the libraries and contribute to the code development. Unfortunately, the literature on the use of open-source software for the computational modelling of AM processes is still very scarce. Most of the research works cited in the previous section do not make use of open-source software and, when they do, little to no detail is given to the reader, making it very hard to draw adequate conclusions. Moreover, a large number of researchers chooses to simulate the process at a macro scale, with a continuous medium powder bed, that provides no information on phenomena at the particle length scale, such as the porosity or sintering evolution. This work is mostly motivated by the absence of enough and detailed information on the topic of SLS simulation, especially within OpenFOAM, as well as the need to develop a model of easy access to conduct the envisaged studies.

Based on the aforementioned information, the main objective for this dissertation is the development of a computational model capable of accurately simulating the SLS process, within an open-source framework. The developed tool should also allow studying the impact of the physical parameters that can be adjusted in the process. To achieve that, on the geometry side, one must represent the powder bed as realistic as possible, with adequate powder particle spatial and size distribution. For the computational model, a solver available in the OpenFOAM library, which was previously studied to assess its adequacy [60], will be further investigated and appropriately adapted to better represent the physical phenomena involved in the SLS process. Towards the end of the project, with the developed computational model, a representative section of the powder bed will be simulated, allowing the studies of the sintering progression and the influence of different underlying parameters.

1.5 Dissertation Outline

The remaining contents of the dissertation are organised into several parts that allow the fulfilment of the outlined objectives for this work. After presenting the motivation and objectives, the SLS process is described in detail in Chapter 2, covering the main mechanisms, phenomena and process variables as well as the associated challenges and limitations. Then, Chapter 3 addresses the process modelling and simulation, based on the state-of-the-art mathematical models and numerical methods employed to describe and solve the associated phenomena, to build a base to critically select the most

adequate computational tools. Afterwards, in Chapter 4, the selected computational tools are described together with the careful characterization of the underlying models being solved. In Chapter 5, the computational model setup is illustrated, comprising the simulation of the representative geometry, mesh generation and material properties, followed by the testing and assessment of the underlying models to ensure that they can correctly represent the process. At the end of this chapter, the proposed case studies are introduced, whose results are presented and discussed in Chapter 6, to evaluate the solver's capabilities and effectiveness to simulate the SLS process. The document ends with Chapter 7, where the main conclusions are drawn and future work is proposed to surpass the identified limitations.

CHAPTER 2 Selective Laser Sintering

2.1 Process Description

As mentioned in Section 1.2, SLS is a process derived from PBF, which implies that it inherits a set of basic principles, such as the three main steps that summarize the process: powder recoating, energy input and material coalescence. A general representation of the SLS process is illustrated in Figure 2.1.

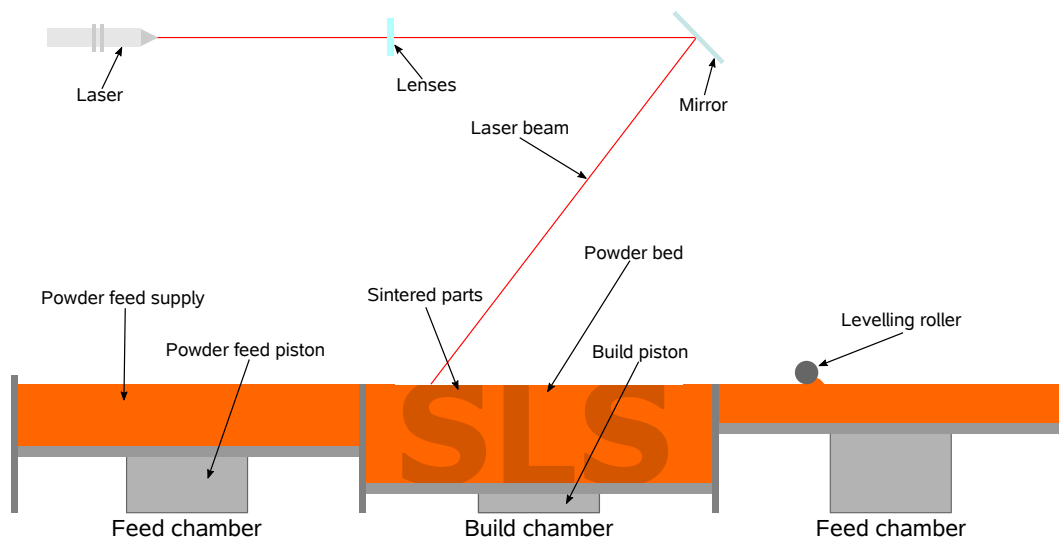


Figure 2.1: General representation of the SLS process.

SLS machines are divided into two main zones, the build chamber, where, as the name suggests, the parts are built, and the feed chamber, that stores the necessary powder for the process and provides it to the build chamber when needed. Two feed chambers are commonly employed so the roller can create a layer starting from any side, removing the need for a return phase. Also, both can collect the excess powder dragged by it, whereas if only one feed chamber is present, an additional zone is required at the opposite side to catch the excess powder. Although possible to use the laser to

melt the material from room temperature, in SLS, the powder is pre-heated to a temperature just a few degrees below its melting point. Besides minimizing the laser power requirements and allowing a faster scanning speed, this reduces temperature gradients between scanned and non-scanned particles, facilitating the fusion between layers and keeping a more uniform temperature on the bed, which helps to prevent defects, such as local shrinkage and thermal distortions caused by non-uniform thermal expansions and contractions [61]. The pre-heating is done in bulk, being achieved through a combination of heat lamps and conductive elements above and around the perimeter of the build and feed chambers, respectively, and is maintained throughout the entire build process. Considering the possibility of the material thermal degradation due to these high temperatures during both the pre-heating and building phases, the process takes place inside a closed chamber filled with an inert gas, generally nitrogen, in order to minimize oxidation.

After the pre-heating phase is complete, the other steps of the process start taking place. Initially, the build piston starts at its highest position and a levelling roller spreads material from the feed supply to the build platform, creating the first powder layer. The amount of material dragged by the roller is always superior to the required for the layer, to assure that it is completely filled. Some machines use a blade instead of a roller to move the powder, however, it has been found that their dragging mechanism produces a less dense powder bed with higher layer surface roughness, when compared to the one obtained with the counter rotating roller [62]. When the layer is complete, a laser beam is directed to the powder bed through a set of lenses and is directed to the desired positions, at a pre-selected speed, with the use of mirrors. The laser type should be selected according to the material present in the bed. For example, for metals, the laser interacts with their electrons, while in polymers the interactions is with the resonant vibration of larger segments of the material molecule. It is known that for aliphatic polymers, the CH₂ segments resonates near 10.6 μm [63], which justifies the wide use of CO₂ laser beams (capable of outputting infrared wavelength from 9 to 11 μm) at that wavelength [64].

As the laser spot moves, it scans the material, providing it enough energy to melt and coalesce with adjacent granules, including the ones on the previous layer (if it exists). The unscanned powder stays in place and works as support for the next layer. The amount of energy provided to the material is crucial to determine the particle consolidation and, consequently, the final part porosity. After the scanning of the present layer is complete, the build piston lowers the powder bed by the thickness of one layer and a new powder layer is spread on top. These operations are repeated until the desired object is fully built and, after that, the heaters are turned off and the part is left to cool inside the machine chamber, so the cooling is as uniform as possible and within an inert ambient, in order to

minimize thermal defects. Although mentioning multiple times that one part is built, multiple objects can be manufactured inside the same bed, as long as the material is the same and there is enough space. A bed with multiple parts is often referred to as part cake. The more parts present in one bed, the more efficient the production process is, so this comes as an advantage. Once cooled, the parts can be removed, cleaned off and, if necessary, subjected to finishing operations.

2.2 Binding Mechanism

SLS is a complex manufacturing technique with various process variables that can be adjusted according to specific needs. However, some adjustments, mainly related to the material and energy density, result in significant differences in the process approach and development, consequently affecting the final part properties. These differences come from the distinct binding mechanisms between the powdered material and, because of that, in order to facilitate communication, different terminologies were given to different technologies according to the predominant binding mechanism. These include four main groups, solid state sintering, chemically induced binding, liquid phase sintering and full melting [65]. It is important to note that, despite being called sintering, most of the approaches do actually melt some of the involved material, as it will be discussed bellow. Independently of the mechanism, because there are no additional forces applied to the powder bed, the coalescence between liquid particles is mainly driven by surface tension forces that pull them together. This phenomenon depends on the material and process parameters and a schematic representation is illustrated in Figure 2.2, where the formation and development of a "neck" between particles is visible.

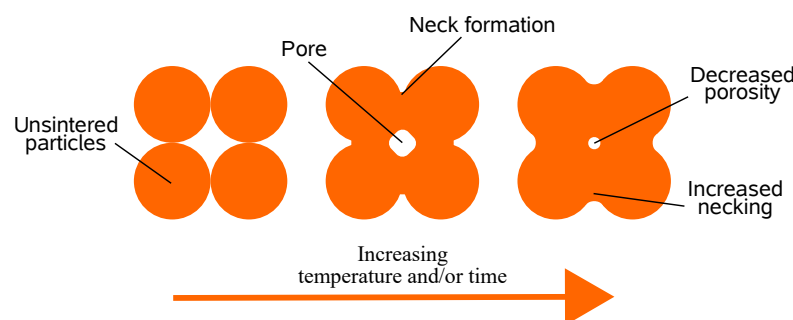


Figure 2.2: Formation of the "neck" between particles.

2.2.1 Solid State Sintering

Solid State Sintering (SSS) is a thermal consolidation process that occurs below the material's melting temperature. It aims at achieving densification by reshaping of the powder in such a way that no liquid is formed. This reshaping is a consequence of reducing energy by eliminating a solid-gas interface and replacing it with a solid-solid one through the diffusion of atoms in the solid state. The tendency of the particles to move to their lowest energy state will "fuse" the adjacent ones together through the formation of a "neck", similar to that shown in Figure 2.2. The "neck" development should be accentuated to minimize porosity, however, the process is very slow because it depends only on diffusion on the solid state so, in order to achieve high sintering rates, it requires either higher temperatures or longer processing times, which comes as a disadvantage, since efficiency both in manufacturing time and energy translate to reduced costs. Because of the negative effects, mainly the time consumption, SSS is only applied to very specific materials, such as ceramics, or for post processing from other techniques [66].

2.2.2 Chemically Induced Binding

This technique is based on thermal activated chemical reactions between two types of powders, or between the powder and a gas, to bind together the particles. It is a fusion mechanism used mainly for ceramics, for example, processing SiC within an atmosphere that contains O_2 , forms SiO_2 that binds itself to the original material, forming a product of SiO_2 and SiC [66]. This technique originates parts with high porosity, making it rely on post-process techniques, such as infiltration or high temperature furnace sintering, to reduce it and obtain appropriate properties [67].

2.2.3 Liquid Phase Sintering/Partial Melting

Liquid Phase Sintering (LPS) is a very versatile mechanism that unifies different types of technologies. Different from other techniques, there are two types of materials with distinct functions, where one, the binder, becomes fully molten and acts as a glue to bind the other, the structural, that remains solid throughout the production process. This approach is useful for cases where the structural material, that contains the desired properties, is hard to process, so another material is used to bind it. The binder and structural materials can be combined in the powder bed in three different ways:

- **Separate Particles** - This approach is the simplest of the three. Creating a good mixture of both structural and binder particles is, in many cases, sufficient to obtain good results. There are, however, some aspects that need to be considered to assure a good quality mixture that will yield parts with good properties. For example, the binder particles must be smaller than the structural ones so the packing is more efficient, leading to less shrinkage, higher density and less porosity. It also increases the binding capability, because the smaller particles will easily fit between the larger ones and, due to their reduced size, melt faster. However, because the laser source moves quickly, there is not always sufficient heat or surface tension forces for the binder to fully flow, meaning that parts formed from separate particles present a higher porosity, thus requiring post processing in a furnace to reduce it [66].
- **Composite particles** - These particles comprise both the structural and binder, which are obtained by mechanically alloying the two materials through grinding cast, extruded or moulded mixtures. This approach aims at reducing the porosity in parts resulting from separate particles and also offers a better surface finish [68]. However, composite particles are also used when the combination of properties from both materials is desired. The most common composite particle is glass-filled nylon, an atypical application where the binder does not act as a glue but instead is reinforced by the structural material, the glass [69].
- **Coated Particles** - The third and last possibility to combine the two materials is to coat the structural particle with the binder material. In the other two cases, as the laser scans the powder bed, the radiation will be absorbed and distributed through all the particles, independent of the material, meaning that the energy is not being focused on the desired constituent, the binder. With coated particles this is not an issue because the binder is always at the particle surface, which is the zone that receives more radiation and, therefore, will absorb more energy and be forced to melt faster. Besides that, the fact that every structural particle is coated with the binder results in an overall better binding efficiency, not only because the surface is the best place for particles to fuse/sinter together, but also because there are no places where the binder is missing due to the particles random mixture, as is seen in the other cases [66].

There are, however, some special cases where there is no distinction between the particles, meaning that there is only one type of material present in the powder bed. For these cases, instead of distinguishing binder and structural particles, there is a distinction of the material physical state. In this situation, "partial melting" is a better suited nomenclature. During the process, when the heat supplied

to the particle is insufficient to fully melt it, only a region will undergo phase change. This allows the molten zone to form a "neck" between particles and act as a binder to the non-molten phase. This is common for materials such as polymers that, due to their low thermal conductivity, will hardly conduct received heat and partial melting of individual particles is possible [70]. Also, because of powder size distribution, different sized particles will require different levels of energy to melt, resulting in fully molten smaller particles while larger ones are only partially melted. Moreover, when alloys are used, one constituent of the alloy might melt before the other, fusing the particles with only a partial melting [66].

2.2.4 Full Melting

Some of the presented techniques yield parts with a significant amount of porosity due to their binding mechanisms principles, mainly the absence of a fully molten layer. The fully melting of the particles came from the need to bypass this defect and produce almost fully dense objects with mechanical properties comparable to those of conventional techniques, while maintaining the advantages of the SLS process. The process that achieves that is commonly referred to as Selective Laser Melting (SLM) (similarly to SLS, it is a patented designation), a technique derived from the SLS process that is exclusive to metals. Despite polymers also fully melting during the SLS process, due to their reduced flow and low thermal conductivity, that allows zones of the same particle to be in different states, they are usually put in the partial melting group, as previously stated. By giving the scanned material enough energy to fully melt, this technique removes the need of mixed material powder beds. The amount of energy provided is also enough to remelt a top portion of the previous layer to assure good adhesion between them. Overall, this procedure is very effective at creating objects with high density as well as assuring a strong bonding between layers [65]. Despite seeming like an upgrade to the other variants, the use of higher energy sources comes with extra challenges, such as part growth and, because the material is now fully molten, extra physical phenomena that may lead to melt pool instability and, consequently, defects and imperfections in the final product [71].

2.3 Polymers in SLS

Polymeric materials represent the developing direction of material science. Over the years, their use has made the people's quotidian much easier, comfortable and convenient. Despite going unnoticed in many applications, polymers are required by many essential industries, such as automotive,

technological and medical. What makes them so attractive and useful are their properties, such as low density, special structures and the ability to be combined with other materials to increase desired parameters. With increasing knowledge on their behaviour, their manufacturing processes are being optimized and higher quality parts are being produced.

The most common used polymers for SLS are thermoplastics because of properties such as low melting temperatures and low thermal conductivity that facilitate the process. Thermosets are unlikely to be used since the SLS method is based on melting a solid material and thermosets, instead of melting, degrade when the temperature is increased. The most used and commercially available thermoplastic for SLS is polyamide-12 (PA12), commonly known as nylon [72, 73]. Its established history for laser sintering applications coupled with ease of processing, relative low cost, when compared to other SLS materials, and mechanical properties, such as tensile strength and elastic modulus, which are now comparable with injection moulded counterparts [74], allow it to prevail even at modern times, where the material availability is more vast. Other variants of the polyamide structure, such as PA6, PA10 and PA11, comprise most of the market remainder, followed by other, less common, polymer families, such as poly(acrylonitrile-butadiene-styrene) (ABS), polystyrene (PS), polycarbonate (PC), polypropylene (PP), high density polyethylene (HDPE), polyetheretherketone (PEEK) and thermoplastic polyurethane (TPU) [72, 73]. It is important to mention that the list of polymers available for the SLS processes is scarcer than other competitive techniques, such as injection moulding, mainly because it is a recent technology and more time is needed to adapt existing materials or find new ones.

Polymers can be distinguished based on their ability to develop crystalline structures, being either amorphous or semicrystalline, as further discussed in Section 2.4.3.3. For the SLS process, semicrystalline polymers (where PA12 belongs to) are more desirable because they yield parts with less porosity and consequent superior mechanical properties [66, 75] and, since most predominant industries require such properties, it is expected that they are more utilized. Besides mechanical strength, semicrystalline polymers are easier to process because they possess much more sharper phase transition points, with well defined melting (T_m) and crystallization temperatures (T_c), which facilitates process control, as mentioned later in Section 2.4.3.2, contrarily to amorphous materials that only present a glass transition temperature (T_g). Amorphous polymers can and have been used [76, 77], but due to previously mentioned difficulties and industry incentives, it is only natural that most of the developments are focused on the semicrystallines.

Apart from being able to crystallize, many other properties are taken into account when assessing

the compatibility of a polymer with the process because being able to use a material is different from obtaining good quality parts from it on a stable and repeatable process. The SLS process is intrinsically complicated and so are polymers, as one might conclude from Section 2.4, which conveys that considering the most important parameters desired for an SLS material is mainly essential and beneficial. Figure 2.3 highlights some of the main factors that limit the selection of a polymer based on various process basis and the complexity behind finding compatibility between both [78]. Some of these properties are discussed with more detail in the next section.

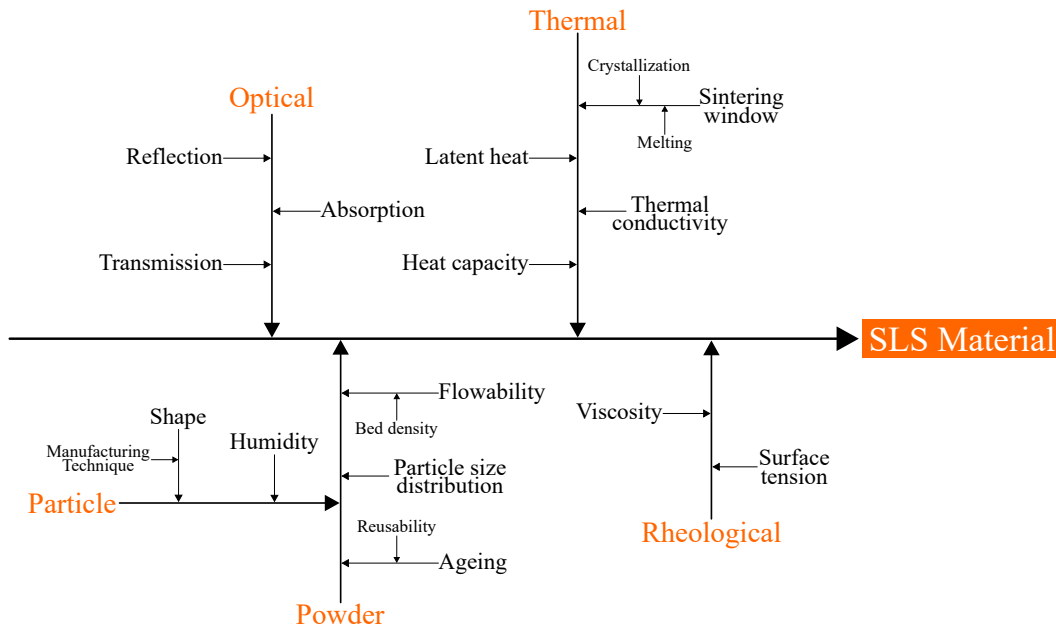


Figure 2.3: Different polymer properties that need to be considered to assess its adequacy to SLS.

2.4 Process Variables and their Influence

As in any manufacturing process, there are variables that influence the process unfolding and its ease of achieving a given standard for final part quality. In theory, it is fairly easy to setup a SLS process, however, in practice, every one of the many process parameters must be accounted for and finely tuned, otherwise the resulting parts will be of low quality, containing many of the possible defects. The process is yet to be fully controllable and, when coupled with the complex properties of the polymers, highly demanding challenges will appear. In order to compete with conventional technologies, objects obtained by SLS must have comparable, or superior, visual and structural properties. Considering that, there are four main criteria in which the part properties depend on [79]:

- The SLS process parameters;

- The properties of the powdered material (particle size, shape and bulk density);
- Material thermal and physical properties (glass transition, melting and crystallization temperatures, specific heat and thermal conductivity);
- Material behaviour during process both in powder and molten state.

Each topic will be discussed in the following sections.

2.4.1 Process Parameters

In laser sintering, the process parameters can be divided into three main groups [80]:

- Laser parameters - Power and spot size;
- Scan parameters - Speed, spacing, count and pattern;
- Build parameters - Layer thickness and build temperature.

Although being distinct features that can be adjusted individually, in practice, because they heavily influence each other, they are adjusted together to optimize the process and final part properties.

2.4.1.1 Laser and Scan Parameters

When setting up the SLS process, one aims at optimizing the energy received by the material particles to make sure they melt and coalesce without degrading, assuring desirable properties in the final product. To calculate the theoretical energy density delivered by the laser to the material in the powder bed, researchers usually use Drexler's energy density (E_D) equation [81]:

$$E_D = \frac{P_L}{v_s H_s d_{\text{layer}}}, \quad (2.1)$$

where P_L is the laser power, v_s the scan speed, H_s the hatch spacing (also known as scan distance) and d_{layer} represents the layer thickness. Based on this equation, one may conclude that many parameters can be adjusted together in order to maximize energy density. As mentioned before, it is much more common to, for example, increase the power and reduce the speed to achieve a certain E_D value, than to simply increase power. That is because, in reality, there are more variables to account for

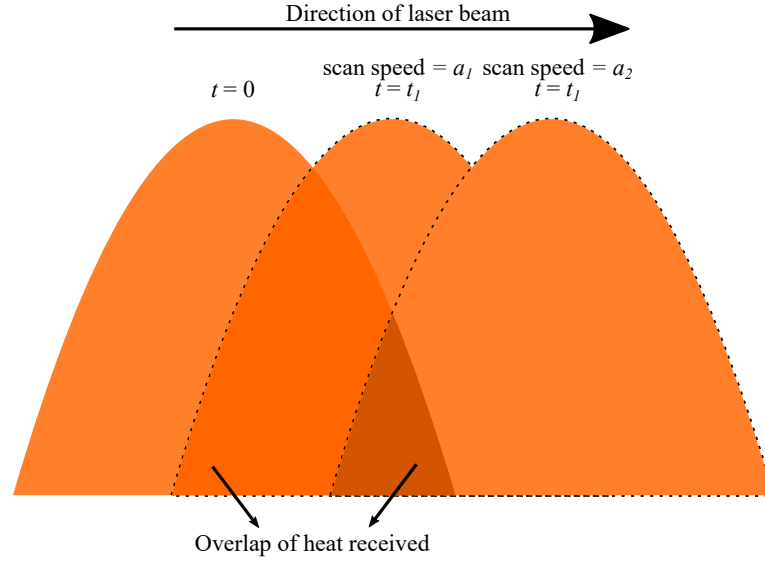


Figure 2.4: Schematic representation of a laser beam with a Gaussian profile moving at two different speeds and its consequent energy overlap on the particles.

and this equation, while useful to get a superficial idea of the volumetric energy received by the layer and the relevant parameters influence on it, is far from a correct approach because of too unrealistic assumptions. For example, the absorptency of the laser energy throughout the layer is assumed to be constant, however, it depends on parameters such as the packing density of the material and attenuates as the laser penetrates it [47]. Also, despite the laser power being constant, its distribution has a Gaussian profile [64], meaning that the heat distribution is not homogeneous and the particles in the target area (centre of the laser beam) will receive more energy than the ones on the edge. The two examples of laser beams moving at different speeds, illustrated in Figure 2.4, evidence that, not only there is an overlap of energy received for a specific region at different points in time, it also differs for different laser speeds, meaning that the equation also fails to consider the movement of the laser and its dependency on time. One last neglected aspect is that, sometimes, the scanning distance is inferior to the laser spot diameter, which means that for subsequent scans, there is always an overlap between the scanned zones and, again, the calculated energy is lower than the real value.

Besides the process parameters discussed in Equation (2.1), there are others that also influence the process unwinding. The present moving heat source, the laser, as it scans the material, creates a temperature gradient at the scanned zone and nearby it. When the immediate next scan line is scanned, some of its heat will affect the previous one, altering its temperature gradient and, consequently, cooling time, which might result in accumulated stresses that induce defects in the final product. These phenomena are inevitable and common to all processes, however researchers are always studying ways to minimize them. In SLS that is achieved by developing a scan strategy, a combination of scan

count, which is the amount of times a layer gets scanned, and scan pattern, to allocate the previously assigned laser parameters into the scanning layer. A good scan strategy should focus not only on minimizing defects, but also on, together with the other parameters, optimize density, micro-structure and mechanical properties [82]. Usually, the contour of the part is scanned and then the area inside of it. In Figure 2.5, some of the most used patterns for the fill part are presented. By changing the pattern, what one is really influencing is the temperature profile observed on the layer and, for subsequent scans, the partial rescanning of the previous one. Typically, long scan vectors in either the x or y axis direction, that can be either uni-directional (Figure 2.5.a) or bi-directional (Figure 2.5.b) are employed. For the former approach, because the vectors always start on the same side, the temperature gradient is the same for each scan line. As for the latter one, the temperature gradient is very small at the end of one vector and beginning of the next, but much more accentuated at the end of one vector and beginning of the previous. The problem with both patterns is that due to the long vectors, the time interval between subsequent scans is increased, which increases undesirable temperature gradients. Also, the temperature gradient increases with the scanning vector size, meaning that larger parts will be even more challenging to build. The island approach, represented in Figure 2.5.c, was developed with the objective of reducing this problem. By scanning small zones of the layer, called islands, the length of the scanning vector is drastically reduced and, consequently, the time interval between adjacent vector is also shorter, therefore, the temperature gradient will be minimized [83]. In addition, it was mentioned before that the energy provided to the layer during the scanning is usually enough to affect the top part of the previous one and reheat it. Generally, the plan for a scan strategy is only for one layer and all the others follow the same pattern (Figure 2.5.e), but it is possible to rotate the pattern in a selected angle, as illustrated in Figure 2.5.d. By rotating intermittently each layer, the resulting parts will benefit from a more even interlayer temperature gradient, which translates into less part distortion and better mechanical properties [84].

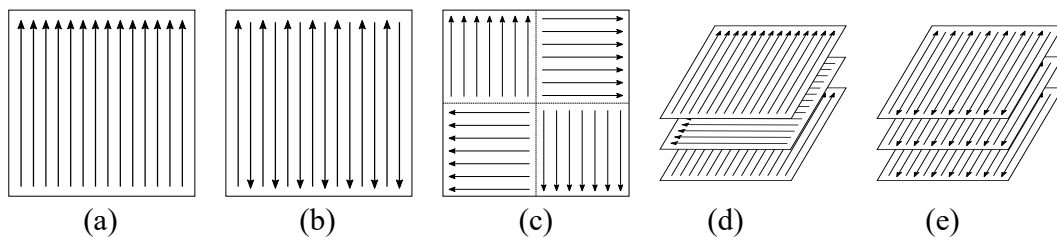


Figure 2.5: Schematic representation of some of the different scan patterns used.

There are other less common strategies being studied, however, going further into the topic exploration falls outside the scope of the present work. Nevertheless, for the interested reader, a more

complete review and discussion can be found in Jia et al., 2021 [83].

2.4.1.2 Build Parameters

Process build parameters comprise the layer thickness and build temperatures to be maintained throughout the process. Generally, they are less complicated to setup due to their more easily predictable influence.

Starting with the layer thickness, it is a parameter that dictates how much the build piston should move downwards after the scan of each layer. It is defined before the machine virtually slices the digital model and, depending on its value, more or less layers are generated. Higher layer thickness values generate less layers for a determined part, which translates to faster production speeds, but sacrifices dimensional accuracy and surface roughness since the resolution is inferior. The maximum value for this parameter is determined by the depth of penetration of the laser energy that, itself, depends on the material absorbency. Each material absorbs a set of electromagnetic wavelengths differently, hence the importance of selecting an appropriate material-laser pair, as stated in Section 2.4.1.1. Usually, the absorbency is measured using thin films with a known thickness, however, in practical cases, the powder bed layer cannot be simplified to such configuration and the penetration depth is always greater due to the empty spaces between particles. Therefore, parameters such as particle size and bed density also influence the penetration depth. Researchers experimentally investigate this depth by scanning and gradually increasing the thickness of each layer and measuring the transmitted power. For PA12, it was reported a consistent absorption of over 90% for a layer thickness of 200 μm [85]. Paired with the penetration depth, the fusion depth, that indicates the limit of laser penetration that also results in particle melting, is usually also evaluated [86]. The knowledge of these values is of great importance to adequately select a maximum layer thickness, which should be smaller than the fusion depth, to assure full coalescence within the layer and a strong connection with the previous one. On the other end, the minimum value for the layer thickness is restricted by the particle size or, in other words, each layer must contain at least one particle of thickness. Generally, the layer thickness is two to three times the average particle size (see Section 2.4.2.1).

The build temperatures are selected according to the material and energy related parameters. All systems are capable of controlling the temperature on the build chamber for the powder bed and its surrounding atmosphere by using a combination of heating elements that surround the powder bed. Some machines have the capability of heating the feed chamber as well, which comes with advantages

and disadvantages. On one side, heating the powder before spreading it reduces the temperature difference between the bed and the fresh layer, which helps reducing temperature gradients and premature cooling. On the other side, the material is held at high temperatures for longer periods, which influences its properties and reusability (more information in Section 2.4.3.4). As explained in Section 2.1, controlling the temperature, as well as pre-heating the powder, is essential for a good process unwinding. Despite being counter-intuitive, most of the energy provided comes from the heating elements and the laser is simply used to overcome the material enthalpy of fusion and thus melting it. Each material and build will have an unique ideal build temperature, but, in general, it is beneficial to select the highest possible temperature that does not promote the consolidation of unscanned particles, to minimize laser power requirements, thermal gradients between scanned and unscanned particles and thermal expansion promoted by the laser [87]. For semi-crystalline polymers, this temperature is a few degrees below T_m and equal, or very close, to T_g , for the amorphous ones. If the build temperature is too high (assuming that it never reaches T_m), the energy required to melt the particles will be so small that non-scanned particles adjacent to scanned ones will still receive enough energy to melt and coalesce. This is often referred to as part growth and is a defect that reduces accuracy and surface finish. Moreover, keeping the powder at even higher temperatures throughout the process further hinders its reusability and also reduces flowability, as mentioned in Section 2.4.3.4 and Section 2.4.2, respectively. Conversely, if the selected build temperature is too low, premature cooling is more prone to happen, accompanied by subsequent contraction and its possible defects (further discussed in Section 2.4.3.3).

It is important to keep in mind that, due to the larger size of the builds and machines, there is always a variation on the temperature despite being set to constant. This variation is attributed to some causes, such as losses of energy from the material to the surrounding elements (machine walls and the naturally generated convection currents in the atmosphere), energy gains from the laser scanned zones and the heating elements inability to provide an even heat source [61]. Although minimal, this variation can have a significant negative impact on the process, especially for polymers with a narrow processing window (see Section 2.4.3.2).

2.4.2 Powder Properties

As suggested by the name of the parent process (PBF), the raw material is used in its powdered form. Although extrinsic, the powder properties interact significantly with intrinsic properties and dictate

the success of the manufacturing process. Selecting and successfully obtaining a powder with the optimal properties is essential to produce consistent, predictable and high quality parts.

2.4.2.1 Powder Manufacture

The majority of polymers are not produced directly in powder form and must be converted to an appropriate particle size prior to sintering. That is usually done via milling/grinding procedures and solvent precipitation, although existing other less common methods that use immiscible blends and melt prilling. Melt-based and mechanical size reduction approaches can be employed for all the materials, while solution-based ones are exclusive for polymers.

Each method results in particles with differences in shape and size distribution, however that is still not well defined or predictable and, unfortunately, it is an area that lacks detailed research studies. Nonetheless, the particles, in terms of shape, fall into three main categories, spherical, potato-shaped and irregular, as shown in Figure 2.6 [78].

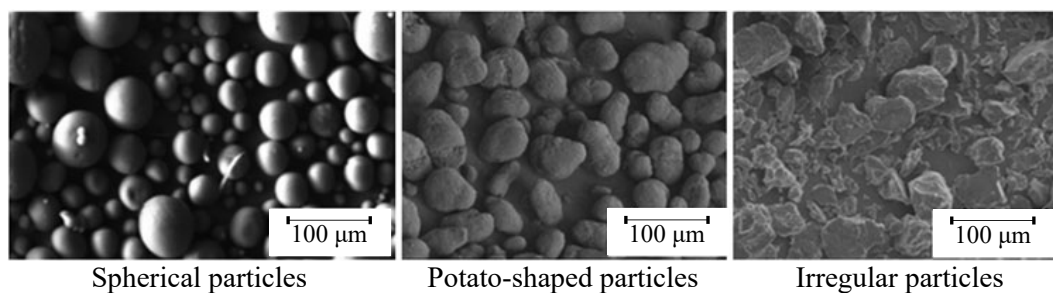


Figure 2.6: Particles obtained by different production technologies [78].

Grinding

Mechanical approaches, such as grinding, are challenging to use with polymers because of their viscoelastic behaviour. Usually, they require cryogenic temperatures to exhibit a more brittle response that allows fracturing, as it is typical in grinding, which increases output and produces a finer product [88]. Because the grinding process converts a large amount of energy into heat, which works against keeping the material cool, other grinding approaches are being evaluated [88]. As of now, despite the efforts, the powders produced by this technique are not recommended due to their non-spherical nature and high portion of small particles that, together, work against their free flow and difficult powder spreading [89].

Solvent Precipitation

The solvent precipitation method is inspired by the dispersion polymerization method and relies on the capability of dissolving together a polymer and a dispersant, creating a solution. The reactive monomer is soluble in the dispersant medium, but the reactant polymer is not, so, when a solvent is added to the solution and the polymer is formed, it immediately precipitates and self assembles into micro-spheres. Another variation is spray drying, where a solution is atomized into a hot drying gas, usually air, evaporating the liquid phase and leaving small particles of the solid phase. In both approaches, the resulting particles have a desirable shape and size distribution [90, 91]. Unfortunately, the solvent precipitation method is not compatible with all polymers and only a fraction can be obtained through this technique.

Immiscible Blends

This approach aims at controlling the morphology of the powder during its manufacturing phase to obtain spherical particles. It works by mixing two distinct polymers in a controlled way to induce a strain rate that will spontaneous form the desired micro-spheres and then, a solvent dissolves the unwanted polymer and the spheres are obtained [92]. Although interesting, this approach is highly dependent on the material properties and imposed parameters, making it challenging to use.

2.4.2.2 Particle Size and Shape Influence

The SLS process has high feedstock requirements, which further restricts the use of many materials. Indeed, one of the reasons that contributes to the short list of available materials in SLS is the need for very specific and challenging to obtain powder properties, such as particles shape, size and size distribution.

Particle Size and Shape

The selected particle size is, generally, as small as possible based on the benefits from denser powder beds and faster sintering. Larger particles can be used, but are less desirable. It is possible to obtain very fine powders, however, regardless of their shape, from sizes lower than 45 μm , static Van der Waals forces start to create agglomerates that oppose their flow and prevents the recoating of a

smooth layer [79], heavily influencing their usability. Therefore, particle size is usually between 45 μm and 90 μm [93]. It is not possible to obtain uniform sized particles and a distribution of sized will always exist so, technically speaking, the powder will have a particle size distribution (PSD). A good PSD should be centred around the desired particle size and not too wide to avoid uneven melting, with smaller particles prematurely fused and larger particles still solid. To assure a good PSD and to diminish problems induced by smaller particles, it is common to filter particles outside the selected range [93]. Despite the mentioned problems, smaller particles can be used when proper treatments to disrupt Van der Waals forces are employed [94]. For particle shape, as expected, spherical (or as spherical as possible) particles are easier to spread and will naturally generate better packing. If the shape is irregular it is very likely to interact and form arches that lead to empty spaces and, consequently, higher porosity [95]. The different shapes are shown in Figure 2.6.

Powder Flow and Bed Density

Particle morphology has a direct impact in the powder deposition phase, also called recoating, that, itself, influences the ease of processing and final product properties [61]. The energy parameters may be more intuitively linked to creating a better product, but having a densely packed bed prior to sintering will minimize void space and, overall, increase desired properties, being a crucial factor for good quality printed parts [79]. Powder flow is a secondary property that depends on the particles size and shape and is generally used to characterize the powder in order to predict its performance. With an increasing flow, density will be higher, so this parameter should be as high as possible. The Hausner ratio is widely considered as a good predictor of flowability [96]. It numerically compares the powder in its highest packed state, often called tapped density, to the resulting packing from a standardized flow condition. Both packing types are illustrated in Figure 2.7. For PA12, this ratio ranges from 0.4 to 0.6, which means that the apparent density is 40% to 60% of the tapped density. This method is often considered insufficiently precise and more PBF related approaches are employed, using modern powder rheometers or other powder spreading machines that aim at mimicking the real process [97]. It is important to note that polymers and metals are submitted to different tests due to their different cohesion levels. Also, despite most of the tests being performed at ambient conditions [96], it should be imperative to consider the higher temperatures in the chamber, that are well above the polymer T_g and promote changes in its properties, which reduce flowability. Differences in humidity should also be measured, as it can promote different levels of agglomeration for hygroscopic polymers [98]. Correctly

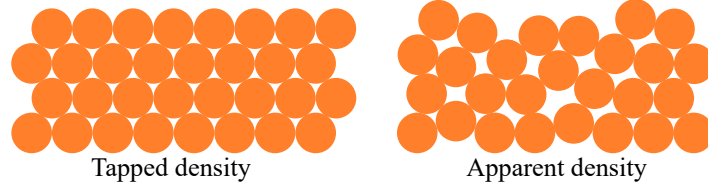


Figure 2.7: Illustration and comparison of tapped and apparent density.

analysing the powder flow and consequent bed density is extremely important because the variations in these parameters are considered to be leading causes for uncertainty and lack of repeatability in the process [99]. Numerous tests have been performed under various conditions for a variety of materials and, overall, it has been observed that flowability increases with the PSD decrease, is improved for larger particles and will decrease in moist environments [98].

2.4.3 Material Thermal and Physical Properties

The chemical structure of the polymer particles is, as expected, very important because it determines other parameters that dictate the usage of the material in the process. Altering it to obtain properties that favour the SLS process is far from trivial, forcing researchers to select materials that naturally fulfil all process needs, which greatly reduces the diversity of polymers that can be employed in the process, as mentioned in Section 2.3.

2.4.3.1 Coalescence

The particles coalescence is one, if not the most, important characteristics of the process. Indeed, numerous process parameters are carefully selected to assure maximum coalescence between scanned particles. Even the employed materials are selected based on their capability to coalesce during the process. If the particles do not fuse together at a sufficiently high rate, the final consolidated part will have poor mechanical properties because of the insufficient adhesion between particles and consequent high porosity. Coalescence takes place after the material is scanned and melts, thus changing to a state with high enough mobility. The amount of mobility that a material has in liquid state determines the rate of coalescence, as shown by the Frenkel model in Equation (2.2) [100]:

$$\left(\frac{x}{r}\right)^2 = \frac{3\sigma t}{2r\eta_0}, \quad (2.2)$$

where x is the growing neck between two particles, r the original particle radius, σ the surface tension in the liquid state, t is the time and η_0 the zero-shear viscosity. This model fails to consider the varying particle radius that results from coalescence, making it only valid for the early stages of coalescence, while the particles spherical shape is preserved. This led other researchers to make adjustments to the model, further increasing its similarity to the SLS particle behaviour [101]. Nonetheless, despite this inaccuracy, the Frenkel model is adequate to assess parameters influence and proves that high coalescence rates are achieved when surface tension is high and viscosity is low.

Surface Tension

At small length scales such as the size of the particles present in the powder bed, surface tension has a prominent impact on the molten material movement, especially because the inertia forces are much smaller. Surface tension can be described as the molecules attractive force, present at the surface of a liquid, towards each other. It is also known as surface energy, although this nomenclature is more correct when referring to the attractive forces between solid molecules, instead of liquid. Any system will always tend to move to its lowest energy state, so, when given enough mobility, that is, when the particles melt, because surface tension pulls surface molecules to each other, the liquid will move towards an equilibrium state that can be represented according to the Young equation [102]:

$$\sigma_{sg} = \sigma_{sl} + \sigma_{lg} \cos \theta, \quad (2.3)$$

where σ_{sg} , σ_{sl} and σ_{lg} are the interfacial surface tensions for solid-gas, solid-liquid and liquid-gas, respectively. An illustration of an arbitrary equilibrium state is shown in Figure 2.8. Based on the equation and the figure, one can predict the behaviour of the liquid if the interfacial surface tensions for the multiple phases are known. For example, assuming that σ_{lg} stays constant, if σ_{sg} increases, then θ will decrease. Contrarily, for a constant σ_{sg} , θ will increase with σ_{lg} . In summary, when σ_{sg} is higher than σ_{lg} , the adhesive forces are stronger than the cohesive forces and the liquid will wet the solid ($\theta < 90^\circ$). On the opposite side, for $\sigma_{sg} < \sigma_{lg}$ the liquid will not wet the solid, but instead tend to form a spherical shape ($\theta > 90^\circ$). For SLS, the predominant surface tension is σ_{lg} because the molten particles will be mostly in contact with others in the same state, therefore, the interaction is only between liquid and gas. Since there are no external forces applied to the melt, the surface tension has to be high enough to overcome its high viscosity and promote coalescence. Also, for the external parts of the layer that are in contact with solid particles, it is not desirable that the liquid material totally wets

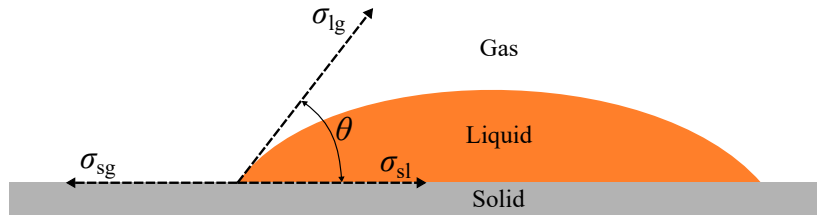


Figure 2.8: Three-phase surface tension equilibrium and resulting contact angle.

the solid particles, so σ_{sg} should not be much greater than σ_g [102]. Researchers have analysed the σ_{lg} in function of temperature and have reported values, for PBF grade PA12 within its melt range, to be between 0.035-0.040 N/m [102].

Viscosity

When in their liquid state, polymers, such as PA12, are very viscous. Since it is desirable to maximize the coalescence rate, according to the Frenkel model, viscosity should be as low as possible. One should note that, in the model, the used viscosity, η_0 , stands for zero-shear viscosity that differs from other values of viscosity for the same material. That is because polymers, being non-Newtonian fluids, have a viscosity that depends not only on temperature [103], but also shear rate [104]. Due to these dependencies, tests performed to evaluate viscosity for a certain process must be done at process equivalent conditions. Polymers exhibit a shear thinning behaviour, typical of pseudoplastics, in other words, their viscosity decreases with increasing shear rate. Considering this, it is not adequate to select a material for SLS, a process where there are no forces applied to the melt, based on results from a capillary rheometer that mimics injection moulding/extrusion conditions. For SLS, cone and plate or parallel discs rheometers are more adequate due to the possibility of much lower, close to zero, shear rates [105]. A polymer viscosity is highly dependent on its molecular weight (M_w) [106] because, contrarily to most materials, polymers are composed of very long molecular chains, that are a combination of many repeating units, and their length is what determines the molecular weight of the material. These chains have a spatial distribution and are able to interact with each other in a similar way that a bunch of wires would. Higher M_w values mean that there are longer chains and, consequently, their interactions, mainly entanglements, are harder to overcome, which, in practical terms, translates into difficulties from the molten material to flow or, in other words, an increase in viscosity. Also, for the same M_w , depending on the entanglement intensity, the viscosity will vary [107]. This justifies the shear thinning behaviour, a consequence of increasing the shear rate, that forces the molecular chains to untangle, hence reducing viscosity. While

low viscosity is desirable for fast sintering, the necessary low M_w to achieve it is not, because it impairs the mechanical properties of the final part. The process applies no external forces to the material so the viscosity is totally dependent on M_w . To circumvent such inconvenience, the polymer is fabricated with an initial low molecular weight that can increase later, during the process. For example, for PA12, this is achieved during its synthesis, more specifically, the ring opening polyaddition of lauryl lactam, where the amino and carboxylic acid end groups are left purposely "unprotected", instead of being chemically terminated [108]. Later, when higher temperatures are achieved inside the build chamber, these groups combine through condensation, increasing M_w [109]. This comes with an advantage of increasing mechanical properties through the later increase in M_w , while maintaining an initial low η_0 for high consolidation. Unfortunately, all the unscanned material in the chamber will also increase in M_w , severely hindering its reusability [110], as further discussed in Section 2.4.3.4.

2.4.3.2 Sintering Window

Particles coalescence is important to assure good final part properties and, as mentioned before, it is not a fast process due to the typical high viscosity of polymers. Obtaining a material capable of sintering at high rates within process conditions is ideal, but it can easily be overthrown if one very important condition, keeping the material in liquid state, is not met. Independently of the selected material, coalescence is only possible in its liquid state, so it is imperative that the scanned particles stay liquid long enough to effectively coalesce. In polymers, for which the solidification temperature is known as crystallization temperature, it is common to have distinct melting and crystallization temperatures. This temperature gap between the onset of melting (T_{OM}) and crystallization (T_{OC}) (illustrated in Figure 2.9) is known as sintering/process/supercooling window. When in between these temperatures (assuming that the polymer is in liquid state and cooling down), solidification/crystallization is not possible and, despite the high viscosity, the material has enough mobility to allow coalescence. Avoiding early crystallization also helps prevent cooling associated defects, as further discussed in Section 2.4.3.3. One material limitation that prevents the use of many polymers in SLS are too narrow, or non-existent, sintering windows. It is challenging to fabricate a part when extremely precise laser parameters and build temperatures are required to avoid premature cooling. Materials that have larger sintering windows are the most desirable since they allow for wider processing temperature ranges, meaning that they are less sensitive to temperature fluctuations and do not require high process precision, allowing the process parameters to be adjusted to optimize other conditions. The lack of a sintering window is one of the reasons why amorphous polymers are less desirable [75].

The compatibility of a new material with the SLS process is often evaluated through a well-known technique for polymer characterization, Differential Scanning Calorimetry (DSC). This technique measures the energy that has to be transferred to, or from, a sample to induce temperature change, thus allowing the identification of thermal transitions, along with their respective enthalpy/entropy. Figure 2.9 presents a schematic representation of a result from a DSC test for a PA12. It shows the various information obtained such as the T_{OM} and T_{OC} but, most importantly, it highlights the interval between them, the sintering window. This large interval, coupled with narrow melting range, for a more centred melting point, low melting temperature, so less energy is required, and a high melting enthalpy, to minimize unwanted sintering from conduction, is why, as mentioned in Section 2.3, PA12 is one of the most common used material for SLS. DSC tests, although also melting and solidifying the sample, are not a totally accurate representation of the SLS process because the heating and cooling rates, contrary to what is observed in the process, are fixed. The values for T_{OM} and T_{OC} are not the same for different heat rates and the material will crystallize sooner when the cooling rates are very low [74]. This results in the narrowing of the sintering window and is the reason why, despite the material still being at a temperature where it should be, theoretically, liquid, after being held at that temperature for long periods (very slow cooling rates), crystallization starts to happen [74].

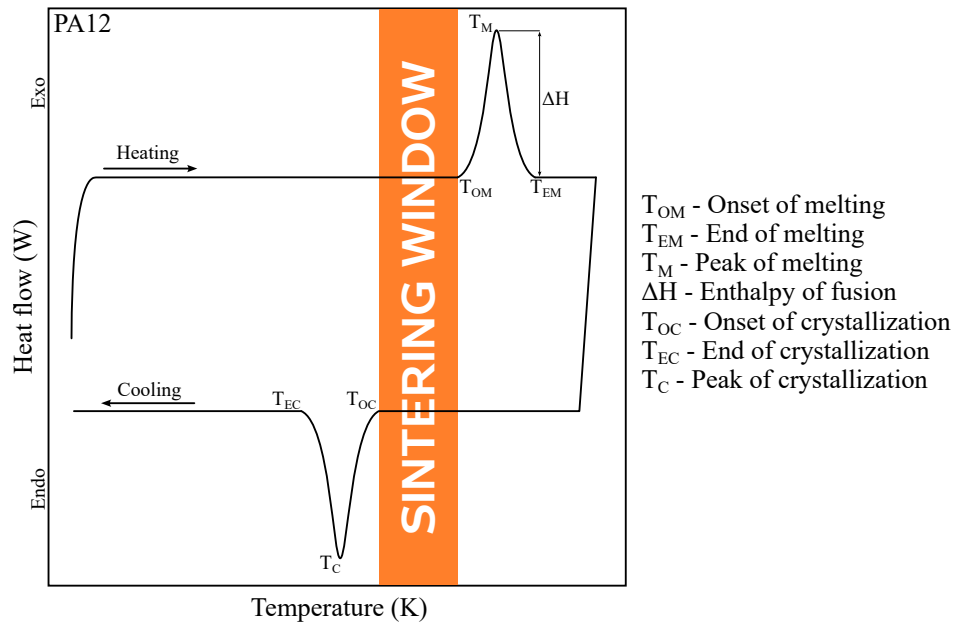


Figure 2.9: Schematic representation of a DSC test for a PA12 highlighting the gap between the melting and crystallization onset.

2.4.3.3 Crystallization

Polymers are composed of long, randomly distributed, molecular chains of various sizes and ramification that interact with each other, as pointed out in Section 2.4.3.1. Some polymers, independently of the conditions, retain such disordered structure upon freezing and turn into an amorphous solid. Others, when certain conditions are met, have the capability of rearranging the chains into a ordered region, known as a lamellae. Since the ordering is not perfect, due to the entanglements that hinder the chains movement, these regions are neither crystalline nor amorphous, but instead a state in between, designated as semicrystalline. The formation of lamellae, known as crystallization, is a kinetically controlled process that depends primarily on nucleation, a phenomenon that occurs in the amorphous region as a result from stimulation of intermolecular forces, which order the chains when cooling the material from its liquid state [111]. Considering that the growth of those organized structures, also called crystallization rate, requires the chains to have enough mobility to organize themselves, for crystallization to take place, temperatures must be above T_g , for enough mobility, and under T_m , so there is nucleation.

In Section 2.4.3.2, the need to suppress crystallization was proved to be essential to assure consolidation between scanned particles and adjacent layers. Besides the interest in keeping the material in a state with higher mobility, to guarantee higher coalescence, delaying crystallization also avoids defects associated with premature cooling. Crystallization is a densification process because the formation of lamellae promotes high levels of organization between molecular chains, which implies that they will occupy less space. When a given amount of polymer densifies, it will, as a consequence, shrink. If during the process, the material reaches temperatures favourable to crystallization, that section will start to crystallize and thus shrink. The problem is not the shrinking itself, but rather it happening prematurely. When a section of the powder bed is allowed to crystallize before it is intended (ideally at the end of the building process), the temperature gradients caused by process conditions, such as the laser, freshly spread powder and heating elements, will cause an uneven material shrinking that will induce internal stress that result in distortion, known as warping and curling [112]. Despite the defects associated with crystallization, semicrystalline polymers are more desirable, when compared to amorphous, because they yield parts with better mechanical properties [66, 75]. Also, crystalline structures are what promote a narrower melting range and subsequent sharper transition from solid to liquid state. Amorphous polymers, due to the lack of organized structures, only possess a glass transition temperature and their viscosity will decrease with increasing temperature for a wide range

of temperatures, making them very challenging to utilize in SLS. Nonetheless, when such challenges are overcome, parts from amorphous polymers can be obtained without severe volume changes and cooling induced defects [113].

2.4.3.4 Reusability

In SLS, there is a large quantity of material that, although required to completely form each layer of the powder bed, does not get consolidated into a part during the manufacturing process. Ideally, the unscanned powder, either being excess in the feeding chamber, or support in the powder bed, would be reused in subsequent builds. Reusing the excess material is desirable from both economic and environmental reasons, because less new and costly "virgin" powder is required and it also significantly reduces material waste. There are materials that, because they suffer minimal to no changes, are considered highly or infinitely reusable, however, for polymers, that is not the case. Throughout the entire part manufacturing process, the material is held at high temperatures, usually well above T_g and very close to its melting point, exposing it to high thermal loads. Polymers, when subjected to such conditions, are vulnerable to chemical and structural changes that heavily influence its properties and consequent behaviour [114, 115], hindering its reuse. The effect of this changes is commonly referred to as ageing and, because it comes from a natural behaviour of the material, it is impossible to avoid.

One example of ageing is the change in viscosity, an important parameter to assure good part quality (see Section 2.4.3.1). At temperatures above T_g , the mobility of the polymer chains is increased and the unstable molecules of the active side groups, known as free radicals, are more prompt to react and attract more molecules to their chain, consequently increasing the molecular weight and number of molecular chains (M_n). The longer the material stays at higher temperatures, the higher the probability of the radicals reacting and the increase in size and number of these chains promotes higher density of entanglements that, ultimately, result in a higher viscosity, as explained in Section 2.4.3.1. This phenomenon, known as post-condensation, is considered material ageing, because it significantly alters its properties, however, some manufacturers utilize it in their favour. The main idea is that the material can start with a low M_w and consequent low viscosity, promoting coalescence, and increase its M_w with time, for better mechanical properties, as described in Section 2.4.3.1. One example is PA12 - PA2200, a widely used polyamide for SLS applications that makes use of postcondensation. Tests show that, despite obtaining the desired initial low viscosity, its increase in M_w promotes an accentuated increase in viscosity over time [109] that make the material reusability very challenging.

Other popular polyamide grades, such as PA12 - Orgasol, keep the M_w values constant by minimizing post-condensation, sacrificing initial viscosity but keeping it constant for much longer [109], making the material much more suitable for reusing. With this approach, even with the side groups terminated during polymerization, ageing still occurs, but at much slower rates and after more cycles [108]. The increase in M_w and consequent viscosity alteration is observed by researchers in the changing of the Melt Flow Rate (MFR), a quick diagnostic tool for evaluating the usability of a powder, used or not [116]. Lower MFR values lead to poorer surface finishing with undesirable effects, such as orange peel, and hamper the particles coalescence [117, 118]. Despite the negative effects, an increase in molecular weight has resulted in particles with slightly increased mechanical properties, meaning that there is a potential benefit of controlled ageing [116].

Another important aspect that influences the polymer properties is the crystallinity. In Section 2.4.3.3, it was mentioned that some polymers have the ability to, between T_g and T_m , develop organized arrangements of molecular chains, thus forming semicrystalline structures. The formation of these structures is not limited to cooling melting material and can also happen by heating the polymer from T_g without melting it [111]. Because the material in the powder bed is held at temperatures within the crystallization range, the solid particles, yet with enough chain mobility, will increase their level of crystallization. The change in the crystalline structure and molecular weight interferes with the enthalpy of fusion of the material [118], which means that the carefully selected energy parameters for the initial powder are no longer optimal [114]. However, these particles, despite their high crystallinity in solid state, once melted, will not be able to achieve high levels of crystallization due to the higher M_w that hinders the ordered chain folding [118].

If the manufacturing process is properly setup and runs smoothly, there should not be any other major properties changes related to ageing. For example, oxidation should be negligible assuming that the atmosphere stays inert during the scanning and cooling phases. In terms of morphology, it has been seen that there are almost no changes in shape or particle size, nonetheless, reused particles appear more cracked than in their original state, probably due to evaporation of solvent or moisture trapped inside them and/or thermal expansion/shrinkage from the processing cycle [118].

Despite the negative effects caused by ageing and how much it hinders the process consistency, due to economic and environmental reasons, it is not desirable to always utilize 100% "virgin" powder. Still, from a process stand point, it is also not adequate to utilize just reprocessed material. A balance between the two types of powder has to be selected to assure good final part properties, with as much

used powder as possible present in the bed. The percentage of new material is indicated through a parameter known as refresh rate that, although specific for each material, is generally a third to a half and the remaining is previously used one [70, 119]. Since the powder ageing is distinct for different sections of the powder bed, because it is exposed to non-identical temperature profiles depending on where it was located, and also increases with the time it was exposed and number of cycles, the refresh rate may vary. In fact, it is common to distinguish used powder based on where it was located, namely the powder bed or the excess chamber, and how long it has been under high thermal loads [117]. In order to properly evaluate how much new material is needed to compensate for the deterioration promoted by the used one, the MFR values of the different used powders is used to guide the preparation of an adequate mixture [117, 119].

CHAPTER 3

Modelling and Simulation

The first step towards the proposed objectives is to find a suitable tool capable of simulating the underlying physical phenomena of the SLS process. Computational Fluid Dynamics (CFD) is a branch of fluid mechanics that comprises a wide spectrum of numerical methods and computer techniques widely used for solving complex flow problems. It provides useful means of simulating transport phenomena such as heat, momentum and mass transfer, making it appropriated for the problem in hands.

Finding analytical solutions to fundamental equations of fluid mechanics is limited to rather simple problems and conditions, often far from the real-world complexity. For that reason, instead of looking for the exact solution, CFD resorts to algorithms that employ numerical methods to determine approximate solutions. Among various methods, three stand out due to their popularity, the Finite Element Method (FEM), the Finite Volume Method (FVM) and the Finite Difference Method (FDM). The first one is widely employed in numerical analysis due to its flexibility, efficiency and the vast amount of available literature [120]. It is generally used for the same problems it was originally developed for, the analysis of solid-state mechanics, but, due to its flexibility, has been also used for fluids. However, its formulation requires special attention to ensure conservative solutions. On the other side, FVM overcomes this problem since it solves the partial differential equations in a conservative form and, when compared to FEM, offers more accurate solutions [121]. The latter, FDM, is simple to formulate and implement, but it can only be used with structured grids, that are harder to adapt to curved surfaces [122]. Various commercial software make use of FVM, as stated in Section 1.3. In particular, OpenFOAM, the software selected to perform the simulations for this work, also uses FVM and, therefore, a more detailed analysis of the method is provided in this work.

When modelling a process, one must take into consideration the computational cost and balance it with the desired accuracy of the model. At this point, it is already known that the SLS process involves a large variety of interacting variables and physical phenomena, making it challenging to study them all simultaneously. In the following sections, the equations that model the most important phenomena are

presented. Since the objective is to study the modelling of a polymer SLS process, some assumptions can be made in order to simplify the model, as it will be discussed further into this chapter.

3.1 Thermal Model

The heat transfer model of the SLS process has to consider both input and output heat fluxes. Since this work aims to study the temperature evolution after the pre-heating phase, the main input heat source, and most of the times the only, is the laser beam. The output heat fluxes occur mainly through convection and conduction and also due to material ablation and radiation losses. Considering that, the energy conservation equation is given by [28]:

$$\rho C_p \frac{\partial T}{\partial t} - \nabla \cdot (k \nabla T) = \dot{Q}, \quad (3.1)$$

where ρ is the material's density, C_p the specific heat, T the temperature, t the time, k the thermal conductivity and $\dot{Q}$ the heat source/sink per unit volume. This equation is used in several SLS models [32, 123] because of its simplicity and the determination of every term in a realistic and computationally efficient way. Despite that, one may notice that this equation does not account for fluid flow. That is because most approaches model the powder bed as a single media [43] and, when coupled with the polymer high viscosity, the convective heat transfer can be neglected. However, for SLM applications, where the metal viscosity is much lower and even at the macro scale, fluid flow effects, such as Marangoni and buoyancy, are noticeable and important. Similarly, when modelling the sintering evolution between particles, considering the fluid flow is necessary. Such consideration transforms Equation (3.1) into [124]:

$$\frac{\partial(\rho C_p T)}{\partial t} + \nabla \cdot (\rho C_p T \mathbf{u}) - \nabla \cdot (k \nabla T) = \dot{Q}, \quad (3.2)$$

where $\mathbf{u}$ is the velocity vector.

3.1.1 Latent Heat

In the previous chapter, it was mentioned that the process parameters have to be carefully selected in order to assure the melting of the scanned particles, therefore, it is important to consider the latent heat associated to phase change. This phenomenon can be implemented in the form of a

modified specific heat term as [125]:

$$C_p = C_{p0} + \frac{\Delta H_m}{\sqrt{\pi}(T_{mf} - T_{ms})} \exp\left(-\frac{(T - T_{ms})^2}{(T_{mf} - T_{ms})^2}\right), \quad (3.3)$$

where C_{p0} is the base specific heat of the material to which the enthalpy heat of fusion ΔH_m is added, distributed between the fusion start and finish temperatures, T_{ms} and T_{mf} , through a Gaussian Law.

Another option would be to consider the latent heat of melting and the heat released during crystallization as a heat sink and heat source, respectively. With this approach, instead of changing the C_p term, the contributions are added to the right-hand side of the energy conservation equation (Equation (3.1)). The latent heat of fusion (heat sink), can be modelled as [126]:

$$\dot{Q}_{\text{sink}} = \delta h \frac{\delta f_{\text{liq}}}{\delta t}, \quad (3.4)$$

where f_{liq} is the volumetric fraction of liquid phase, calculated as [126]:

$$f_{\text{liq}} = \frac{(T - T_{\text{sol}})}{(T_{\text{liq}} - T_{\text{sol}})}, \quad (3.5)$$

where, given the range of melting temperature $\Delta T = T_{\text{liq}} - T_{\text{sol}}$, its value varies from 0, when $T \leq T_{\text{sol}}$ to 1, when $T \geq T_{\text{liq}}$, always satisfying $f_{\text{liq}} + f_{\text{sol}} = 1$. δh is the total absorbed latent heat over a melting temperature range for a two-phase medium given by $\delta h = H_{\text{liq}} - H_{\text{sol}}$, with H representing the enthalpy of both liquid and solid constituents [127]. Both terms are calculated as [127]:

$$H_{\text{liq}} = \rho_{\text{liq}} \int_{T_{\text{sol}}}^T C_{p_{\text{liq}}} d\theta + \delta H, \quad (3.6)$$

$$H_{\text{sol}} = \rho_{\text{sol}} \int_{T_{\text{liq}}}^T C_{p_{\text{sol}}} d\theta, \quad (3.7)$$

where ρ_{liq} , ρ_{sol} , $C_{p_{\text{liq}}}$ and $C_{p_{\text{sol}}}$ are the density and specific heat of the liquid and solid material, respectively, and δH is the reference enthalpy for the liquid. Oppositely, in the cooling phase, polymers crystallize and release energy, acting as a heat source that can be modelled by the following equation [32]:

$$\dot{Q}_{\text{source}} = \rho_{\text{sol}} \frac{\delta \alpha_c}{\delta t} \Delta H_c, \quad (3.8)$$

with α_c representing the crystallinity rate and ΔH_c the crystallization enthalpy. The term $\frac{\delta \alpha_c}{\delta t}$ accounts for the evolution of the relative degree of crystallization as a function of time and temperature and can be described by the Nakamura's model [128]:

$$\frac{\delta \alpha_c}{\delta t} = n K(T) (1 - \alpha_c) \left[\ln \left(\frac{1}{1 - \alpha_c} \right) \right]^{\frac{n-1}{n}}, \quad (3.9)$$

where n is the Avrami index that depends on the growth geometry of crystallites and $K(T)$ is the non-isothermal crystallization rate. $K(T)$ can be related to n and determined by the following expression [129]:

$$K(T) = \ln 2^{\frac{1}{n}} \left(\frac{1}{t_{1/2}} \right), \quad (3.10)$$

with $t_{1/2}$ representing the half crystallization time for a defined isothermal temperature. The determination of that time can be expressed by the Hoffman-Lauritzen theory [130]:

$$\left(\frac{1}{t_{1/2}} \right) = K_0 \exp \left(\frac{-U}{R(T - T_\infty)} \right) \exp \left(\frac{-K_G(T + T_0)}{2T^2(T_0 - T)} \right), \quad (3.11)$$

where K_0 is a temperature independent constant, U is the activation energy of the crystallization transport with the universal value of 6270 J/mol, R the universal gas constant that is equal to 8.314 J/mol/K, T_∞ is the temperature at which the crystallization transport finishes, that takes the value of $T_g - 30K$, K_G is a parameter related to the nucleation characteristics and T_0 is the equilibrium melting point. All the unknown parameters are determined by means of DSC.

3.1.2 Laser Beam

When modelling the laser beam it is important to formulate an equation that takes into account its shape and power distribution. From Section 2.4.1.1, it is known that the types of laser beams employed into SLS processes have a Gaussian intensity profile and a circular shape, hence only the radius being mentioned as a parameter. When treated as a surface heat source, following such conditions, the power intensity of the laser Q_{LB} can be expressed as [28]:

$$Q_{LB}(x, y) = \frac{P\eta}{2\pi\sigma^2} e^{\frac{x^2+y^2}{-2\sigma^2}}, \quad (3.12)$$

where P is the laser beam power and η the material absorptivity, that can be calculated, if the material reflectivity (λ) is measured experimentally, with $\eta = 1 - \lambda$ [131]. The position on the surface is given by coordinates x and y and the point of highest intensity, the centre of the beam, corresponds to the origin of this local coordinate system. The standard deviation σ indicates the variation in intensity along the laser spot radius r_{LB} . One should aim at obtaining an adequate distribution throughout the radius, where the maximum intensity is at the centre and decays to values close to zero as it approaches the periphery, so the selection of σ cannot be random. To assure a good distribution that fits inside the spot radius, researchers define the standard deviation proportionally to it, as to satisfy $\sigma = r_{LB}/2$. This slightly modifies Equation (3.12) into [51, 131]:

$$Q_{LB}(x, y) = \frac{2P\eta}{\pi r_{LB}^2} e^{-2\frac{x^2+y^2}{r_{LB}^2}}. \quad (3.13)$$

This way, when the distance to the centre is equal to r_{LB} , the intensity value is reduced by a factor of e^2 of the maximum value. This approach also makes the equation easier to read, because it replaces the standard deviation of the intensity distribution with the laser radius, an easier parameter to define. However, from previous attained information, it is known that the laser has the ability to go through the material and, in fact, it is necessary that it does, to effectively melt the entire thickness of the scanned powder. Modelling the laser as a surface 2D heat source is simpler, but far from realistic, since, in reality, it exhibits a volumetric 3D behaviour. In this case, the energy attenuates as it penetrates the material because it is being absorbed until, eventually, it extinguishes. This behaviour follows the Beer-Lambert equation, which is an exponential equation that can be written as [44, 132]:

$$Q(z) = Q_0 e^{-\alpha z}, \quad (3.14)$$

where Q is the transmitted laser power in the thickness direction z , Q_0 the surface heat source from Equation (3.13) and α the extinction coefficient, with the term $e^{-\alpha z}$ representing the exponential decay along the powder bed thickness. From this equation, the energy distribution function can be written as [132]:

$$q(z) = Q_0 - Q_0 e^{-\alpha z}, \quad (3.15)$$

that, after a simple derivation, is transformed into [132]:

$$q(z) = \alpha Q_0 e^{-\alpha z}. \quad (3.16)$$

If Q_0 is replaced with the surface heat source from Equation (3.13), the equation of the volumetric heat source is obtained and it can be added to Equation (3.1), in the $\dot{Q}$ term, as a heat source:

$$Q_v(x, y, z) = \alpha \frac{2P\eta}{\pi r_{LB}^2} e^{-2\frac{x^2+y^2}{r_{LB}^2}} e^{-\alpha z}. \quad (3.17)$$

Besides the energy distribution of the beam, given by a Gaussian distribution along the radius, and the energy absorption of the material modelled by the Beer-Lambert equation, more phenomena are present during the scanning phase. One popular modelling approach for the laser beam is to discretize its domain into a finite number of rays so that each individual one can interact with intersecting media. Such consideration is important because the laser is an electromagnetic wave and it is well known that they suffer an alteration in their direction when they encounter a change in medium, as illustrated in Figure 3.1.

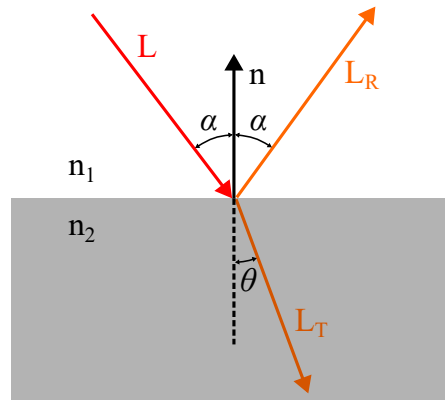


Figure 3.1: Laser reflection and refraction when changing media.

Looking at this illustration, the initial ray, represented by the vector $\mathbf{L}$, when changing medium, from n_1 to n_2 , gets terminated and two new rays, $\mathbf{L}_R$ and $\mathbf{L}_T$, are cast in different directions, representing the reflection and refraction suffered by $\mathbf{L}$, respectively. The reflected ray, since its travelling in the same medium, has the same angle α as its former ray relatively to the surface normal $\mathbf{n}$. Because the initial ray gets split in two, each one will keep a portion of its total energy E_I . By using the Fresnel equation for

unpolarized light and non-magnetic media, the portion of reflected energy E_R can be calculated as [47]:

$$E_R = \frac{1}{2} \left[\left(\frac{n_1 \cos \alpha - n_2 \cos \theta}{n_1 \cos \alpha + n_2 \cos \theta} \right)^2 + \left(\frac{n_1 \cos \theta - n_2 \cos \alpha}{n_1 \cos \theta + n_2 \cos \alpha} \right)^2 \right] E_I. \quad (3.18)$$

The remaining non reflected energy, given by $E_T = E_I - E_R$ is refracted through the new medium. Contrarily to the reflected ray, the refracted one travels in a different medium at which the wave will propagate at a different velocity, causing an alteration on the angle in relation to $\mathbf{n}$. The newly formed refraction angle θ can be determined using Snell's law [47]:

$$\sin \theta = \frac{n_1}{n_2} \sin \alpha, \quad (3.19)$$

where n_1 and n_2 are the refractive index of each medium.

3.1.3 Heat Losses

During the building process, the energy losses from the powder bed to the environment are minimal when compared to the energy absorbed by the material. Nonetheless, they exist in the form of convection to the surrounding air, emissive radiation and, even less pronounced, conduction to the external walls and material ablation. The process takes place inside an insulated chamber where there are not many elements taking heat away from the system, which leads to some models neglecting their contribution to the energy equation [133]. However, despite being common practice to ignore energy losses when modelling small sections, because the errors scale with time and volume, it is recommended to consider them for larger builds. In that case, even only the predominant losses are considered, with conduction and ablation being frequently ignored, and the heat transfer coefficients for convection and radiation are grouped together as [134]:

$$h = (h_{\text{conv}} + h_{\text{rad}}). \quad (3.20)$$

The heat loss flux is then modelled according to Newton's Law of cooling [44, 134]:

$$-k \frac{\partial T}{\partial n} = h(T_s - T_\infty), \quad (3.21)$$

where $-k \frac{\partial T}{\partial n}$ is the convective heat flux, with n being the surface's unit normal vector, h is the integrated heat transfer coefficient and T_s and T_∞ the surface and environment temperatures, respectively. The

values for h_{conv} can be determined as a function of the Nusselt number (Nu):

$$h_{\text{conv}} = \frac{Nu k}{L}, \quad (3.22)$$

where k/L represents the conductive heat transfer, with L being the characteristic length of the specimen. If the scanned, molten zone is considered a horizontal plate, Nu itself can be determined by [135]:

$$Nu = 0.54 Ra^{0.25}, \quad (3.23)$$

where Ra is the Rayleigh number that is given by the product of the Prandtl (Pr) and Grashof (Gr) numbers ($Ra = Pr Gr$), which can be calculated as [135]:

$$Pr = \frac{C_p \mu}{k}, \quad (3.24)$$

$$Gr = \frac{g \rho \beta (T_s - T_\infty) L^3}{\mu^2}, \quad (3.25)$$

with g being the gravitational acceleration, μ the viscosity and β the volumetric expansion coefficient. All the variables present in these equations are for the fluid properties only. In a different manner, the heat flux due to radiation is described by the Stefan-Boltzmann Law [134]:

$$q_{\text{rad}} = \varepsilon \sigma (T_s^4 - T_\infty^4), \quad (3.26)$$

with ε being the surface emissivity and σ the Stefan-Boltzmann constant with the value of $5.6710^{-8} \text{ W/m}^2 \text{ K}^4$. The radiation is then linearised and treated as an effective heat transfer coefficient so it can be utilized in Equation (3.20) and fit into Equation (3.21) format [134]:

$$q_{\text{rad}} = h_{\text{rad}} (T_s - T_\infty), \quad (3.27)$$

$$h_{\text{rad}} = \varepsilon \sigma (T_s + T_\infty) (T_s^2 + T_\infty^2). \quad (3.28)$$

It is important to note that there is no energy loss to the air in the beginning of the scanning process, right after the pre-heating, because the air was also pre-heated, so there is a thermal equilibrium. The

major aforementioned heat losses from the material only start to happen after the laser starts to scan the powder bed and the system thermal equilibrium is disturbed.

3.2 Linear Momentum

Most works on the simulation of SLS processes only consider the temperature profiles, sintering depth and phase change, whereas mass transfer is neglected [28]. However, sometimes researchers want to study the sintering evolution between scanned particles or, in the case of SLM, motion effects caused by differences in density in the liquid phase. In these cases, it is imperative to consider the momentum, that is given by Newton's Laws of motion, and assure its conservation. Compared to energy or mass, momentum is harder to deal with because it is represented as a vector, meaning that it has both magnitude and direction. Considering that, the governing equation for the momentum conservation is given as [124]:

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = \nabla \cdot (\mu \nabla \mathbf{u}) - \nabla p + \rho \mathbf{g} + \mathbf{F}, \quad (3.29)$$

with μ representing the viscosity and g the gravitational acceleration. F accounts for extra forces that are considered depending on the modelling approach. For metals, these additional forces generally comprise buoyancy, the Darcy's term and surface forces including capillary forces (surface tension), thermo-capillary forces (Marangoni effect) and recoil pressure [136, 137]. Again, for SLS with polymer applications, due to the high viscosity and consequent reduced flux, the model is generally simplified and F only accounts for surface tension, that is modelled as [138]:

$$F_\sigma = \sigma \kappa \nabla \alpha, \quad (3.30)$$

where σ is the surface tension constant value, α the phase fraction and κ is the mean surface curvature, that can be calculated as [138]:

$$\kappa = -\nabla \cdot \mathbf{n} = -\nabla \cdot \left(\frac{\nabla \alpha}{\|\nabla \alpha\|} \right). \quad (3.31)$$

3.3 Continuity Equation

The continuity equation, also known as mass conservation equation, describes the conservation of mass in the problem. The change of mass over time, represented as $\frac{dm}{dt}$, refers to the mass that can flow into and out of the control volume. Physically, volume can also change overtime, but considering that the control volume is constant, mass is related to it by density. This denotes that the change in mass depends on the density and on the flux of mass through the volume as the following equation describes:

$$\frac{dm}{dt} = \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}). \quad (3.32)$$

The models for the SLS process generally consider the involved fluids to be incompressible in the calculation process, therefore, because the density is constant, the term $\frac{\partial \rho}{\partial t}$ is equal to 0 and the continuity equation only depends on the sum of the converging/diverging fluxes that, too assure mass conservation, must also be 0:

$$\nabla \cdot \mathbf{u} = 0. \quad (3.33)$$

3.4 Powder Deposition

The powder deposition is one of the main steps of the process. It occurs once for every layer and is the first action towards its fabrication. In Section 2.4.2, powder properties such as their shape, size and size distribution were associated with the quality of the powder bed, more specifically, its density and absence of voids. Since the powder bed is the foundation of the process, it is imperative to assure that it stays consistent and of good quality throughout various processes. Even with the other parameters optimized, if the base of the process is defective, so will be the final part.

When simulating the SLS process, some approaches consider the powder layers as a continuum domain with mixed properties between material and air, according to the expected powder bed density [43]. Modelling the layer this way is much easier, but it only provides information on the macroscopic scale. Nonetheless, it is a much simpler way to determine temperature profiles and sintering/melting depth. However, this approach, due to its excessive geometry simplification, does not provide any information on phenomena that happens at particle length scale, such as porosity and

sintering evolution. More useful data could be obtained if the powder bed was modelled as realistic as possible, but this requires the mesh to be much more refined, in order to accommodate many small particles, and the coupling of different simulation methods.

The powder bed is considered a granular material, more specifically, a group of numerous discrete solid particles that interact with each other through collisions and/or other interaction types dispersed over a domain. From a macroscopic scale, a granular material cannot be assigned to a state type, such as solid or liquid, because none can represent the complete behaviour of the group of particles. Despite the particles being solid, because of their small size, when under certain conditions, such as being dragged by a roller over the powder bed, they behave similar to a fluid, hence researchers studying powder flowability (see Section 2.4.2.2). Moreover, under highly agitated systems, groups of particles can behave as a gas, as seen daily with dust particles in the air. That is why, when grouped together, small solid particles form a granular material. Modelling the interaction of the particles during their deposition over the powder bed cannot be done with mesh based methods, such as the ones mentioned in the previous sections, and, instead, a meshless approach is employed in the form of a suitable numerical method. The Discrete Element Method (DEM) is widely used for particle simulations. In fact, it was developed in 1979 by Cundall [139] to simulate the behaviour of granules such as soil. DEM discretizes granular media in a way where each particle is a single element and then calculates the interactions between them at a microscopic level, so one can observe the influence of such interactions at a macroscopic level. This method requires a contact detection strategy, interaction Laws and time discretized equations of motion that govern the particle displacements.

The motion of individual particles is governed by the Newton-Euler Laws of motion, while the interactions between them are calculated using a variety of models suitable for a particular geometry and material behaviour, considering the necessary forces. As in any simulation, there are numerous models available [140] and their selection may vary according to process conditions, materials and/or the complexity desired. Generally, DEM approaches consider translational and rotational motion and the governing equations are given by [141]:

$$m \frac{d^2 \mathbf{P}}{dt^2} = \sum (\mathbf{F}_n + \mathbf{F}_t + \mathbf{F}_c) + m \mathbf{g}, \quad (3.34)$$

$$I \frac{d\omega}{dt} = \sum (T - R_f), \quad (3.35)$$

where m is the mass of the particle, $\mathbf{P}$ the position vector, $\mathbf{F}_n$ and $\mathbf{F}_t$ are the contact forces in

the normal and tangential direction, respectively, $\mathbf{F}_c$ the cohesion forces and $\mathbf{g}$ is the gravitational acceleration. Moreover, I is the inertial moment, given by $I = 0.4mr$ [141], ω is the angular velocity, T is the torque that the particles exert on each other due to contact forces and R_f is the rolling friction. In Figure 3.2, a schematic representation of the force diagram, with the relevant forces for the powder bed simulation, for two contacting particles with radii r_1 and r_2 and masses m_1 and m_2 , is illustrated. The torque T from other contacting particles is given by [24]:

$$T = rF_t, \quad (3.36)$$

and the rolling friction is calculated as [141]:

$$R_f = \mu r \mathbf{F}_n \bar{\omega}, \quad (3.37)$$

where r is the particle radius, μ is the friction coefficient for the sliding friction and $\bar{\omega}$ is the angular velocity unit vector. The cohesion forces $\mathbf{F}_c$ are based on the Johnson-Kendall-Roberts (JKR) cohesion theory. They represent attractive forces due to van-der-Waals effects and are essential for a correct powder bed simulation because of the particles small size, as discussed in Section 2.4.2.2. They are implemented as $\mathbf{F}_{JKR}$ [142]:

$$\mathbf{F}_{JKR} = -4 \sqrt{\frac{\pi a^3 E \lambda}{2(1 - \xi^2)}} \vec{e}_n, \quad (3.38)$$

where a is the contact radius, E the Young's modulus, λ is the surface energy density and ξ represents the Poisson's ratio. The contact forces $\mathbf{F}_n$ and $\mathbf{F}_t$ are calculated based on the Hertz-Mindlin contact theory as [143]:

$$\mathbf{F}_n = (\kappa_n \delta_n^{3/2} + \zeta_n \mathbf{v}_n) \vec{e}_n, \quad (3.39)$$

$$\mathbf{F}_t = \min(\kappa_t \delta_t + \zeta_t \mathbf{v}_t, \mu \mathbf{F}_n) \vec{e}_t, \quad (3.40)$$

with δ_n , given by $\delta_n = r_1 + r_2 - \bar{r}_{12}$, where the last term is the distance between the centre of the particles, representing the compression of colliding particles in the normal direction and δ_t the deformation between particles in the tangential direction at the contact points. The velocity is represented as v_n and v_t and the unit vectors as $\vec{e}_n$ and $\vec{e}_t$, both in the normal and tangential direction,

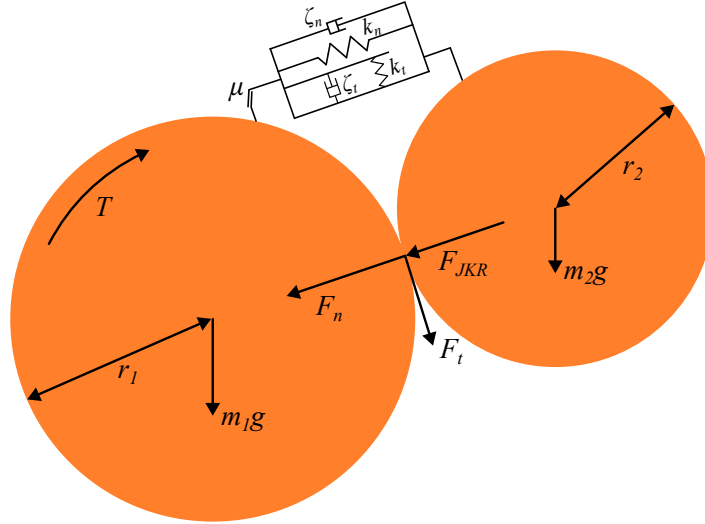


Figure 3.2: Schematic representations of the forces between two particles

respectively. In Equation 3.40, if the left term inside the parenthesis is larger than the right one, which represents the maximum friction between the two particles, tangential slide will occur [144]. Since after slipping, no extra force is being applied, because friction has been overcome, it is necessary to numerically limit the values of F_t to those of the maximum friction, hence the notation to select the minimum value between the two. The effective stiffness (κ) and damping (ζ) coefficients in both the normal (n) and tangential (t) directions are calculated according to the material properties as [24]:

$$\kappa_n = \sqrt{\frac{r_1 r_2}{r_1 + r_2}} \frac{2E}{3(1 - \xi^2)}, \quad (3.41)$$

$$\zeta_n = \sqrt{\frac{m_1 m_2}{m_1 + m_2}} \frac{\ln e}{\sqrt{\ln^2 e + \pi^2}} \sqrt{\frac{5\kappa_n}{2}}, \quad (3.42)$$

$$\kappa_t = \sqrt{\delta_n \frac{r_1 r_2}{r_1 + r_2}} \frac{2E}{(2 + \xi)(1 - \xi)}, \quad (3.43)$$

$$\zeta_t = \sqrt{\frac{m_1 m_2}{m_1 + m_2}} \frac{\ln e}{\sqrt{\ln^2 e + \pi^2}} \sqrt{\frac{5\kappa_n}{3}}, \quad (3.44)$$

where e represents the restitution coefficient that needs to be considered because all particles are assumed rigid, so a relation between their velocity before and after impact is needed.

3.5 Finite Volume Method

The FVM is a discretization method for numerically solving a single, or a system, of Partial Differential Equations (PDEs) expressing the conservation of one or more quantities. PDEs are used as models in a variety of scientific fields describing the relation between partial derivatives and/or their derivatives (temperature, pressure, density, etc.) as function of variables within the domain, such as space and/or time.

When attempting to simulate a process, its physical domain must be modelled considering the different materials, dimensions and interactions. Following that, the physical phenomena involved must also be modelled to create a set of governing equations. These equations will then be discretized by FVM over the domain that must also be discretized. At the end, a system of linear algebraic equations is obtained and solved to find the governing equation numerical solutions.

3.5.1 Domain Discretization

The numerical solution of a PDE consists on calculating the values of a dependent variable at specific points within the domain. To obtain those points, the domain must be subdivided into a finite number of discrete non-overlapping elements, often referred to as control volumes (CV) or cells, generating a computational mesh. The mesh is classified based on several properties, commonly the cell shape, structure and orthogonality. In FVM, cells can be of various convex polyhedral shapes and are completely bounded by faces that are shared between two cells, with the exception of boundary faces. For the discretization step, information about the elements connectivity volume, centroid, number of faces and their respective centroid, area and normal vector is needed.

3.5.2 Equation Discretization

Due to their complexity, the three governing equations (mass, momentum and energy) in the form of PDEs, presented in the previous sections, cannot be usually solved by analytical methods. In order to obtain a solution, a numerical method, in this case the FVM, is employed, discretizing the PDEs over each mesh CV into a set of algebraic equations, as to assure a relation that connects the value of a variable in a cell to its neighbours. This process is often referred to as numerical discretization.

General Transport Equation

The governing equations employed in this study can be represented by a general transport equation for a field ϕ that stands for any scalar given, as shown in Table 3.1 [145]:

$$\frac{\partial(\rho\phi)}{\partial t} + \nabla \cdot (\rho \mathbf{u} \phi) - \nabla \cdot (\Gamma_\phi \nabla \phi) = S_\phi, \quad (3.45)$$

where Γ_ϕ represents the diffusion constant.

Table 3.1: Representation of the governing equations as a general transport equation.

Conservation equation	Temporal derivative	Advective term	Diffusion term	Source term
Mass	$\frac{\partial \rho}{\partial t}$	$\nabla \cdot (\rho \mathbf{u})$		
Momentum	$\frac{\partial(\rho \mathbf{u})}{\partial t}$	$\nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u})$	$\nabla \cdot (\mu \nabla \mathbf{u})$	$-\nabla p + \rho \mathbf{g} + \mathbf{F}$
Energy	$\frac{\partial(\rho C_p T)}{\partial t}$	$\nabla \cdot (\rho C_p T \mathbf{u})$	$\nabla \cdot (k \nabla T)$	$\dot{Q}$
General transport	$\frac{\partial(\rho \phi)}{\partial t}$	$\nabla \cdot (\rho \mathbf{u} \phi)$	$\nabla \cdot (\Gamma_\phi \nabla \phi)$	S_ϕ

Gauss Divergence Theorem

Equation (3.45) is the starting point for computational procedures in FVM. To find its solution, the method relies on the integration of the equation over the control volume. By doing so, the following equation is obtained [146]:

$$\int_{t^{n-1}}^{t^n} \left[\int_{CV} \frac{\partial(\rho\phi)}{\partial t} d\mathbf{x} + \int_{CV} \nabla \cdot (\rho \mathbf{u} \phi) d\mathbf{x} - \int_{CV} \nabla \cdot (\Gamma_\phi \nabla \phi) d\mathbf{x} \right] dt = \int_{t^{n-1}}^{t^n} \left(\int_{CV} S_\phi d\mathbf{x} \right) dt. \quad (3.46)$$

where $\mathbf{x}$ is the (x, y, z) vector. With all the terms rewritten as integrals over the entire CV, the Gauss divergence theorem can be applied to transform the volume integrals of the terms into surface integrals. This theorem states that the divergence of a vector $\mathbf{a}$ over the volume of the cell CV is equal to the component of that vector in the direction normal to the cell surface $\mathbf{n}$, integrated over the surface area,

or boundary of the control volume, ∂CV [146]:

$$\int_{CV} \nabla \cdot \mathbf{a} \, d\mathbf{x} = \int_{\partial CV} \mathbf{n} \cdot \mathbf{a} \, d\mathbf{x}. \quad (3.47)$$

Because the surface area of the cell is the sum of the area of its faces, the theorem can be further simplified to:

$$\int_{\partial CV} \mathbf{n} \cdot \mathbf{a} \, d\mathbf{x} = \sum_f \left(\int_f \mathbf{n} \cdot \mathbf{a} \, d\mathbf{x} \right) \approx \sum_f \mathbf{S}_f \mathbf{a}, \quad (3.48)$$

where $\mathbf{S}_f$ represents the vector normal to the face with a magnitude equal to its area.

Diffusion Term

The discretization of the diffusion term is done by applying the Gauss' divergence theorem over it, obtaining [146]:

$$\int_{CV} \nabla \cdot (\Gamma_\phi \nabla \phi) \, d\mathbf{x} = \int_{\partial CV} \mathbf{n} \cdot (\Gamma_\phi \nabla \phi) \, d\mathbf{x} \approx \sum_f \mathbf{S}_f \cdot (\Gamma_\phi \nabla \phi)_f = \sum_f (\Gamma_\phi)_f \mathbf{S}_f \cdot (\nabla \phi)_f, \quad (3.49)$$

with the subscript f representing the values at the face. One should note that this approximation is only valid if Γ_ϕ is a scalar. The calculation of the gradient of ϕ at the face is done with the following expression [147]:

$$\mathbf{S}_f \cdot (\nabla \phi)_f = |\mathbf{S}_f| \frac{\phi_N - \phi_P}{|\mathbf{d}|} + \mathbf{k} \cdot (\nabla \phi)_f, \quad (3.50)$$

where ϕ_N and ϕ_P are the scalar values at the neighbour and current cell center, respectively, and the second term is a non-orthogonal correction. For orthogonal meshes, only the first term is considered since the second term vanishes. A geometric illustration of the equation is shown in Figure 3.3.

The discretization of the boundary faces is slightly different and also depends on the condition imposed on the boundary. Similarly, the calculation of the non-orthogonal correction depends on the selected method, however, the detailed explanation of all the discretization approaches falls outside the scope of the present work. Nonetheless, more information can be found in the book by Moukalled et al. [147].

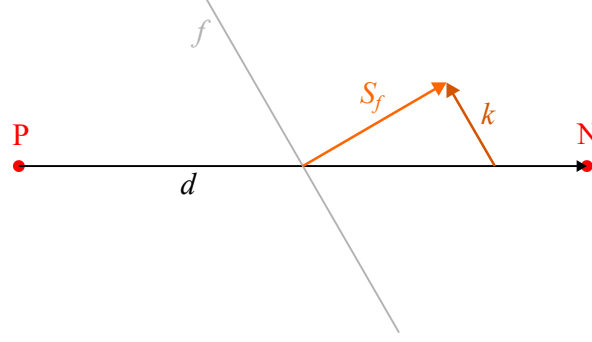


Figure 3.3: Discretization of the diffusion term in a non-orthogonal mesh.

Advective Term

The advective term is discretized in an alike manner by also applying the Gauss divergence theorem [146]:

$$\int_{CV} \nabla \cdot (\rho \mathbf{u} \phi) d\mathbf{x} = \int_{\partial CV} (\rho \mathbf{u} \phi) d\mathbf{x} \approx \sum_f \mathbf{S}_f \cdot (\rho \mathbf{u} \phi)_f = \sum_f \mathbf{S}_f \cdot (\rho \mathbf{u})_f \phi_f, \quad (3.51)$$

with $\mathbf{S}_f \cdot (\rho \mathbf{u})_f$ representing the mass flux F that passes through the faces. The value of ϕ at the face is generally calculated from its values at the cell centres of the two cells P and N that share the face. Several different schemes can be employed for this calculation, with a simple one being the Central Difference (CD) illustrated in Figure 3.4. This scheme linearly interpolates the value at the centre of the face from the values at the centre of the cells, as expressed by the following equation [147]:

$$\phi_f = f_x \phi_P + (1 - f_x) \phi_N; \quad (3.52)$$

where f_x is the interpolation factor given by $\frac{fN}{PN}$, or, in other words, a weighing factor based on the distance from the face centre to the centre of each cell.

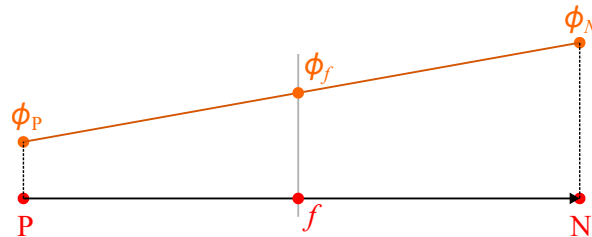


Figure 3.4: Interpolation of the dependent variable at the face using the CD scheme.

Source Term

The source terms do not fit in the other previously mentioned categories, as it is the case for, for example, the laser beam. They are commonly linearised in terms of the dependent variable ϕ and divided in two parts, one that is treated explicitly (S_E) and other implicitly (S_I) [147]:

$$S_\phi(\phi) = S_E + S_I \phi. \quad (3.53)$$

After integrating this new expression over the CV, the following equation is obtained:

$$\int_{CV} S_\phi(\phi) dV = S_E V_P + S_I \phi_P V_P, \quad (3.54)$$

where V_P is the volume of the cell and ϕ_P the value of the unknown at the center of the cell.

Rate of Change Term

Thus far, the discretization of the spatial terms was presented. In a general form, for all of them, it transforms the volume integrals into surface ones from where discrete expressions that relate cell values are obtained. Applying the same procedure to the rate of change term results in [147]:

$$\int_{CV} \frac{\partial(\rho\phi)}{\partial t} dV = \left(\frac{\partial\rho\phi}{\partial t} \right)_P V_P. \quad (3.55)$$

With all the terms discretized, the general transport equation can be re-written as:

$$\int_{t^{n-1}}^{t^n} \left[\left(\frac{\partial(\rho\phi)}{\partial t} \right)_P V_P + \sum_f F \phi_f - \sum_f (\Gamma_\phi)_f \mathbf{S}_f \cdot (\nabla\phi)_f \right] dt = \int_{t^{n-1}}^{t^n} (S_E V_P + S_I V_P \phi_P) dt. \quad (3.56)$$

This equation is referred to as semi-discretized because, despite containing the discretization of the spacial terms, it lacks the discretization of the temporal ones. To obtain the discretization of the latter terms, the temporal contributions are integrated in time. Assuming a Crank-Nicholson time discretization, for example, a linear variation of ϕ along time, the following equations for the rate of change term and the remaining others, respectively, are obtained [146, 147]:

$$\int_{t^{n-1}}^{t^n} \left(\frac{\partial(\rho\phi)}{\partial t} \right)_P dt = \rho_P^n \phi_P^n - \rho_P^{n-1} \phi_P^{n-1}, \quad (3.57)$$

$$\int_{t^{n-1}}^{t^n} \phi(t) dt = \frac{1}{2}(\phi^{n-1} + \phi^n)\Delta t, \quad (3.58)$$

where ϕ^{n-1} denotes the value from the previous time step, t^{n-1} , and ϕ^n the value at the time step being solved, t^n . By applying these notions to Equation (3.56), it is finally fully discretized in the popular Crank-Nicholson form [147]:

$$\begin{aligned} \frac{\rho_P^n \phi_P^n - \rho_P^{n-1} \phi_P^{n-1}}{\Delta t} V_P + \frac{1}{2} \sum_f F(\phi_f^{n-1} + \phi_f^n) - \frac{1}{2} \sum_f (\Gamma\phi)_f \mathbf{S}_f \cdot ((\nabla\phi)_f^{n-1} + (\nabla\phi)_f^n) \\ = S_E V_P + \frac{1}{2} S_I V_P (\phi_P^{n-1} + \phi_P^n). \end{aligned} \quad (3.59)$$

System of Equations

From the analysis of the above equation, one can conclude that, in order to solve the problem and determine the present values of ϕ at the faces, the contributions from all the terms are required as well as the values of ϕ from the previous iteration. That leads to an algebraic equation with the following form for each CV [146, 147]:

$$a_P \phi_P^n + \sum_f a_N \phi_N^n = S_P \quad (3.60)$$

with a_P representing the coefficient for the CV of interest, a_N the the coefficient for the neighbour cells and S_P the source terms. By assembling the equations for all computational cells, a system of equations is obtained in the form of:

$$[\mathbf{A}]\{\phi\} = \{\mathbf{b}\} \quad (3.61)$$

where $\{\phi\}$ contains the unknown values that will be calculated, $[\mathbf{A}]$ is a sparse matrix composed of the the a_P coefficients on the diagonal, and the coefficients of the neighbour cells, a_N , on the off-diagonal positions. Lastly, $\{\mathbf{b}\}$ represents the source terms. By solving this system of equations, the solution of the mass, momentum and energy conservation equations can be obtained and the main variables values are calculated.

After reviewing the modelling of the most important phenomena in the SLS process, a set of computer based techniques, also known as computational tools, are necessary to analyse and solve the equations. For the problem in hands, multiple tools are required, since different methods need to be employed. The different tools for each method, along with their process compatible models, will be described in the following sections.

4.1 OpenFOAM

Open-source Field Operation And Manipulation or, in short, OpenFOAM [148], is a free open-source software used to solve a multitude of complex CFD problems. It is composed of a vast library of models and equations written in C++ programming language, which has been used and greatly expanded throughout the years by a growing community of contributors across most areas of engineering and science. Since 2004, it has been mainly developed by OpenCFD, with two major releases every six months that include customer sponsored developments and contributions from the community. The software is compatible with most Linux distributions, mainly Ubuntu, but it can also be used on other major operative systems, such as Windows and macOS, through the Docker [149] or WSL [150], that provides a self-contained Linux subsystem with a compatible environment for it. Since OpenFOAM base version lacks a graphical user interface, executing commands is done through the command prompt and the visualization of the data is done through post-processing with external software, for example, ParaView [151].

4.1.1 General Case Structure

Each OpenFOAM case consists of a directory structure that contains specific files, stored in specific folders, that are required to run the simulation. Because OpenFOAM is a toolbox that contains many solvers, according to the application, particular files might be needed. Figure 4.1 represents the general structure of a case.

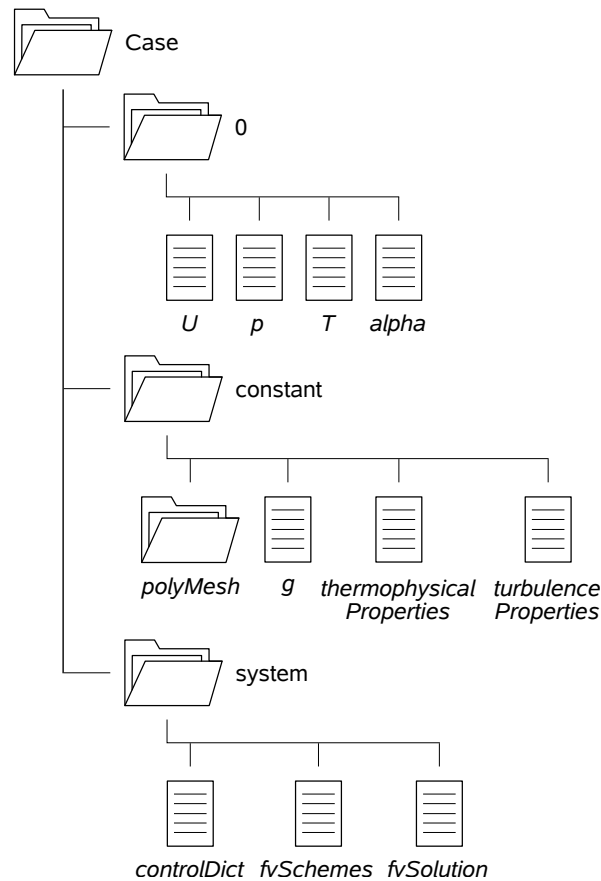


Figure 4.1: General case directory structure.

Time directories

The time directories contain the solution fields for specific time-steps and are generated during the simulation, apart from the initial data (usually in the 0 folder), which contains the initial and boundary conditions for the simulation. The variables are specified using the International System of Units (SI) and are displayed as **SI [kg m s K mol A cd]**. Typically, this folder contains information regarding the velocity (*U*), pressure (*p*), temperature (*T*) and phase (*alpha*). For multiphase problems, each phase requires an *alpha* file. The simulation can also be started from a subsequent time.

Constant directory

This directory contains files that allow characterization of the problem physics, as well as the computational mesh. The mesh is stored in the *polyMesh* folder, distributed between multiple files that contain information on the points and the faces that they form when orderly connected, as well as the boundary faces that are generally grouped into patches used when specifying boundary conditions. Most solvers require additional information on gravity (g), the presence or absence of turbulence and the thermophysical properties of the involved phases, such as density and specific heat.

System directory

The system directory contains files that dictate how the problem should be solved. The three included in Figure 4.1 are mandatory to every case. The *controlDict* file is for the specification of more general settings, such as the simulation time-step, start and end time, how often a time-step solution should be written to the case directory, what format the data files have and, for transient solvers, the maximum Courant number. The other two files are for controlling simulation options related to the methods. *fvSchemes* contains the necessary information related to the discretization schemes for the governing equations differential terms, namely how each equation is integrated with respect to time, how the gradient of each field is calculated, the discretization of the divergence, Laplacian and surface-normal gradient terms and how the interpolation from cell-centred values to face-centred values is computed. *fvSolutions* is where the user specifies the controls for the solution and algorithm, such as residual control. Another optional files consist of mesh generation dictionaries, such as *blockMeshDict*, subdivision of the domain for parallel processing with the *decomposeParDict* and, very frequently used, *setFieldsDict*, which allows the user to set a region anywhere in the domain with a specific value.

4.1.2 icoReactingMultiphaseInterFoam Solver

The icoReactingMultiphaseInterFoam solver was originally released with OpenFOAM version 1806 [152]. It is a subcategory of the multiphaseInterFoam solver that, itself, is based on the parent solver interFoam, which solves the continuity and momentum Navier-Stokes equations for two fluids with a phase fraction that is tracked resorting to the volume of fluid algorithm [153]. multiphaseInterFoam follows the same principles, but for multiple incompressible fluids, tracking phase fraction, while also

considering surface tension and contact-angle effects for each phase [154]. Being a subcategory of these solvers, `icoReactingMultiphaseInterFoam` shares many features, but was complemented with additional functionalities. For instance, it allows the user to choose the thermodynamic model for each phase, but the main assumption of the shared fields among the phases from `interFoam`, namely velocity, pressure and temperature, remain. The solver supports mass and heat transfer between different phases of the same material, similar to the ones on which it is based, but also allows it between different phases of the different materials.

Among the many solvers present in the OpenFOAM library, the `icoReactingMultiphaseInterFoam` was selected because it meets the modelling requirements for the SLS process presented previously, such as modelling the polymers phase change, considering fluid flow and taking into account interactions between multiple phases, including interface tension forces. The solver also contains a laser radiation model capable of modelling a volumetric heat source, following a Gaussian distribution, that attenuates as it passes through the material. Previous work was also done to explore and assure the solver capability to simulate the SLS process [60], which further reinforces its selection to model the problem of interest.

4.1.2.1 phaseProperties

Being a multiphase solver that accounts for multiple interactions between the different phases, a dictionary for the specification of the models for certain interactions alongside their parameters is needed. For this solver, that dictionary is located in the constant folder and is named *phaseProperties*. The available models that can be indicated on it are described below.

Phase models

The solver comprises three basic phase models:

- `pureMovingPhaseModel` - adequate for flowing phases (fluids).
- `multiComponentMovingPhaseModel` - used for multi-component fluids (fluid mixtures)
- `pureStaticSolidPhaseModel` - meant for solids.

For the SLS process modelling, the adequate models should be `pureStaticSolidPhaseModel` for the powder particles in solid state and `pureMovingPhaseModel` for regions where the temperature

surpasses a defined value, transforming the solid into a liquid. Selecting a model for a phase in this dictionary will later dictate what properties are necessary to provide for each phase, for example, when specifying a phase as a solid, the viscosity is not requested.

Mass transfer models

Mass transfer models should be selected when two previously specified phases can be transformed into each other due to phase change. The solver has only two options, the kineticGasEvaporation model, used for condensation and evaporation, and the Lee model, for melting and solidification applications. Since the polymer particles can be either in solid or liquid state, melting and solidifying as the process evolves, the relevant model is the latter.

The Lee model [155] assumes that the phase change occurs at a constant pressure and at a quasi-thermal equilibrium state and that it mainly depends on the difference between the interfacial cell and saturation temperatures. Because the Lee model is used more often, in the literature, for condensation and evaporation, the following equations are slightly adapted so it is easier to understand them in this context. However, the original ones can be found in some recent studies [156–158].

For melting, when $T > T_{\text{activate}}$, the mass transfer rate from solid to liquid $\frac{dm_{sl}}{dt}$ is:

$$\frac{dm_{sl}}{dt} = C\rho_l\alpha_l \frac{T - T_{\text{activate}}}{T_{\text{activate}}} \quad (4.1)$$

and for solidification, when $T < T_{\text{activate}}$, the mass transfer rate from liquid to solid $\frac{dm_{ls}}{dt}$ is:

$$\frac{dm_{ls}}{dt} = C\rho_s\alpha_s \frac{T_{\text{activate}} - T}{T_{\text{activate}}}. \quad (4.2)$$

In both equations, ρ_l , ρ_s , α_l and α_s are the density and phase volume fraction for the liquid and solid material, respectively, T_{activate} is the activation temperature, commonly referred to as saturation temperature (T_{sat}) and C is a constant value that represents an empirical coefficient, called the mass transfer intensity, which is used to adjust the phase change rate. Some researches have found that small values of C result in a significant deviation of the interface temperature from T_{sat} and that increasing this value helps reduce that. Used values range from 0.1, for flow boiling, to 7.5×10^5 , for micro-channel condensation. Such information and more on this topic, with several references, can be found in Lee et al. [158]. In the solver adaptation of the model, C also works as a switch, meaning that if it has a positive value, only melting can occur at that temperature, otherwise, there is only

solidification. Both phase change directions are possible if both are individually specified.

Inter-phase porosity models

The inter-phase porosity models purpose is to add an artificial momentum source on or next to the interface between the two phases, which can influence the behaviour during phase change, mainly for solidifying or melting. The solver has only one model available for said function, named *VollerPrakash* after its creators [159, 160]. This model aims to solve the major problem of assuring a null velocity as the liquid region turns into solid. The approach is to treat the cells in which phase change is occurring as pseudo porous media, where the porosity (λ) ranges between 1 and 0 for a fully liquid or solid cell, respectively, with an intermediate value during phase change. Most applications of convection-diffusion phase change numerical methods have been made to isothermal phase change problems, assuming that the material is pure and has a very well defined phase change temperature. Despite being a general method that can handle such situation, the model was developed to also consider the "mushy" region created during the phase change of materials, such as alloys and polymers, that, for example, melt over a temperature range, which implies that the evolution of latent heat has a functional relationship with temperature ($\Delta H = f(T)$), as opposed to pure materials where there is a step transition. Modelling the "mushy" zone is more challenging since it represents a solid-liquid mixed state of the material.

The *VollerPrakash* implements two source terms in the momentum balance equation, S_u and S_b . The first term is given by [159]:

$$S_u = -A\mathbf{u}, \quad (4.3)$$

with $\mathbf{u} = (u, v, w)$ representing the velocity vector in the "mushy" zone, governed by the Darcy law:

$$\mathbf{u} = -\frac{\kappa}{\mu} \nabla P, \quad (4.4)$$

where κ is the permeability, given as a function of porosity by $\lambda = 1 - F_s$, with the latter term being the solid fraction, whereas A works as an intensification factor for the velocity calculated in Equation (4.4). For an isothermal problem, where the porosity approach is typically a numerical "fix", any increasing function for this term would be suitable, however, for a "mushy" zone, where a porous zone indeed exists, one should resort to physics to assure a proper form for the A term. The well-known

Carman-Koseny equation [161], derived from the Darcy Law, shows the relation between the cell gradient of pressure, porosity and velocity:

$$\nabla P = -\left(\frac{C(1-\lambda)^2}{\lambda^3}\right)\mathbf{u}. \quad (4.5)$$

This equation suggests that A should be represented as [159]:

$$A = -\left(\frac{C(1-\lambda)^2}{(\lambda^3 + q)}\right), \quad (4.6)$$

with q being a constant, which takes very small values, introduced in the equation just to avoid division by 0. The value of C , another constant, depends on the morphology of the porous media. A will increase from 0 to large values as F_s in the cell increases from its lowest liquid value of 0 to its highest fully solid value of 1. This defines the source term as negligible in the liquid region and the momentum equation is given in terms of the actual fluid velocities. However, as phase change starts to occur and the "mushy" zone is formed, the source term's influence increases along with A . The values of A increase in such a way that the value of the sources overpass the transient, convective, and diffusive terms contributions and the momentum balance equation approximates the Darcy Law (Equation (4.4)). Following this equation, as F_s approaches 1, the velocity will tend to 0 and along high values of A , this source term will dominate all other terms in the momentum balance equation and force the predicted superficial velocities to approach zero.

The second source term added by the model, S_b , is a buoyancy term implemented to induce natural convection and it adds momentum only in the vertical direction. It assumes that the Boussinesq approximation is valid, which means that the density is constant in all terms except a gravity source term, and is described as [159]:

$$S_b = \frac{\rho g \beta (h - h_{\text{ref}})}{C_p}, \quad (4.7)$$

where β is the thermal expansion coefficient, h is the sensible heat and h_{ref} its reference value.

Surface Tension Models

To include surface tension forces, the user must specify the value for a pair of phases. The solver is only capable of treating the surface tension as a constant continuum surface force. The equation that

models this phenomena is based on the general approach for considering surface tension forces, which is illustrated in Equation (3.30).

4.1.2.2 Radiation model

As mentioned previously, the availability of an adequate radiation model was one of the motivations to select this solver. It uses the Discrete Transfer Radiation Model (DTRM) to simulate a collimated radiation flux that allows for interaction between the laser and the participating media [152]. DTRM based methods work by discretizing the laser into multiple rays that will interact with the domain. Using such methods allows for the consideration of reflection and refraction of the individual rays, however, one should find a balance between the number of rays and their respective interactions, as ray tracing tends to be computational expensive.

In the laser dictionary, *radiationProperties*, it is possible to adjust the available laser parameters, as well as some additional models. Within the available parameters, there is the laser power, expressed in Watts, direction, indicated by a vector, and position, which can be either constant or vary with time to simulate the laser target movement. The shape of the beam is a circular disk with a user defined radius and the distribution of rays inside the laser periphery is given by a polar division of that disk, with *nTheta* number of particles in the theta direction, and *nr* particles along the radial direction. The power distribution of the laser can be either manually defined, uniform, or, similar to the reality, have a Gaussian distribution. It is also possible to define how the laser interacts with each phase, with the *localDensityAbsorptionEmission* model, allowing for different phases to have different emission and absorption coefficients. Both the power distribution and emission coefficients are treated similar to the common approaches in literature, as described in Section 3.1.2. The power intensity follows the same formula as Equation (3.12) and the user defined radius is not used directly into it, but instead to truncate the Gaussian distribution.

In this dictionary, the user can also select a model to account for the reflection. One of them is named *Fresnel* and has similar but more complex approach than the commonly employed models in the literature, which were described in Section 3.1.2. This model calculates the reflectivity by decomposing the wave into two linear components that are vibrating within the plane of incidence ρ_P and its normal ρ_N , represented by [162]:

$$\rho_N = \frac{(n_1 \cos \alpha - p)^2 + q^2}{(n_1 \cos \alpha + p)^2 + q^2}, \quad (4.8)$$

$$\rho_P = \frac{(p - n_1 \sin \alpha \tan \alpha)^2 + q^2}{(p + n_1 \sin \alpha \tan \alpha)^2 + q^2} \rho_N, \quad (4.9)$$

where n_1 is the refractive index of the medium of the incident ray and α is the angle between the incident ray and the surface normal. The total reflectivity ρ is given by $(\rho_N + \rho_P)/2$. Lastly p and q are calculated as [162]:

$$p^2 = \frac{1}{2} \left[\sqrt{(n_2^2 - k_2^2 - n_1^2 \sin^2 \alpha)^2 + 4n_2^2 k_2^2} + (n_2^2 - k_2^2 - n_1^2 \sin^2 \alpha) \right], \quad (4.10)$$

$$q^2 = \frac{1}{2} \left[\sqrt{(n_2^2 - k_2^2 - n_1^2 \sin^2 \alpha)^2 + 4n_2^2 k_2^2} - (n_2^2 - k_2^2 - n_1^2 \sin^2 \alpha) \right], \quad (4.11)$$

with n_2 being the refractive index of the remaining medium and k_2 is the absorptive index, also known as the imaginary part of the index of refraction. This implies that, instead of just mentioning the refractive index of each medium, for the absorption medium, one has to specify the complex index of refraction m in the form of $m = n_2 + ik_2$.

4.2 LIGGGHTS

LIGGGHTS [56] is an open-source Discrete Element Method particle simulation software whose code is written in C++ programming language. The software's name is an acronym that stands for LAMMPS Improved General Granular and Granular-Heat Transfer Simulations, where LAMMPS is a widely used simulator in the Molecular Dynamics (MD) field. LIGGGHTS uses LAMMPS as a platform, making improvements on it by moving from MD to DEM through the addition of characteristic features of DEM such as simulation of contact and cohesion forces, rolling friction and heat conduction between particles. LIGGGHTS is being developed with the goal of being used in industrial applications, hence the possibility to import complex CAD geometries, utilize moving meshes and include a variety of particle insertion options.

4.2.1 Input Script

Contrary to OpenFOAM, LIGGGHTS reads all simulation parameters from a single input script, all written by the user. The input file must follow a specific structure because the software will read from

top to bottom, executing commands in the order that they appear, so they must be arranged correctly.

A typical LIGGGHTS input script has 4 parts:

1. Initialization
2. Atom/particle definition and insertion
3. Settings
4. Run the simulation

The last two parts can be repeated to allow the user to change settings during the simulation and then resume it, without having to restart it and create two separate files.

Initialization

Before defining the particle system, it is necessary to first set a group of parameters that will define the simulation. These parameters are set with the following commands:

- ***units*** - This command determines the units of all quantities specified in the input, log and dump files. The options available range from units for very small scale problems, such as *metal* and *electron* that, for example, measure distance in Angstroms and Bohr, respectively, to more common units such as *si* (International System) and *cgs* (centimetres grams seconds). For the powder bed simulation, since the particles size are at the micrometer scale, a convenient units command in LIGGGHTS would be *micro*, which gives the following main units:
 - mass = picograms (pg)
 - distance = micrometers (μm)
 - time = microseconds (μs)
 - temperature = Kelvin (K)
 - charge = picocoulombs (pC)
 - electric field = volt/micrometer ($\text{V}/\mu\text{m}$)
- ***dimensions*** - A simulation can be either in two or three dimensions. The user must specify with the corresponding numbers, 2 or 3.

- ***newton*** - This allows the user to turn *on* or *off* Newton's third law for pairwise and bonded interactions.
- ***processors*** - For parallel runs, the users are allowed to manually define how processors are mapped in a 3D logical grid. LIGGGHTS allows such customization with the command *processors Px Py Pz*, where a number of processors should be selected for each axis. By default, this command does not have to be specified and the software automatically manages the distribution.
- ***boundary*** - This command is used to set the style of the boundaries for the simulation box in each dimension. The command is defined as *boundary x y z*, where letters will replace the directions according to the user specification. A single letter assigns the same style to both faces in that direction. The periodic style, given by the letter *p*, means that the particles that exit through one face of the boundary box will enter through the opposite. This is the only style that allows such behaviour. For style *f*, the position of the boundary is fixed and particles that enter in contact with it will be deleted. The last two, *s* and *m*, are for shrink-wrapped, which indicates that the boundary will move to encompass the particles in the dimension and the latter will limit the face displacement to a minimum value, set by the user.
- ***atom_style*** - Allows the user to define the type of atoms used in the simulation and determines the attributes that are associated to them. It affects what quantities are stored by each atom and communicated between processors. For very small scale problems, such as molecular, it is useful to consider data such as bonds and angles between them, but in the powder bed scale, that information is not pertinent. The options *sphere* and *granular* are the best suited since they consider, for each particle, its velocity, mass and diameter.
- ***atom_modify*** - This parameter is optional and only used for molecular simulations. It allows the modification of previously selected properties of the *atom_style*.

Definition

Defining the particles is an essential step for the simulation, since the software is a particle simulator. In LIGGGHTS there are three ways to define the particle/atom system. In case the user has a specific particle system and wants to study its evolution, the software can read an initial set of parameters from a data file. Another similar option is to use a restart file, that contains the

information from a previous simulation. However, because most users use the software to also generate the particles, it is also possible to insert them from a plane. The insertion command requires the specification of a particle distribution template and then randomly generates the particles into the simulation box with a user specified velocity vector. As for the particles themselves, it is possible to customize their shape, size and properties such as density, Young's modulus and Poisson's ratio. Furthermore, the restitution, sliding friction and rolling friction coefficients between pairs such as particle-particle or particle-geometry can also be customized.

Settings

Once the main simulation parameters and particle system have been defined, a variety of simulation specific setting can be introduced. In this phase, the user must specify the simulation region, the time step and variables for particle insertion time, geometry movement and other parameters of the same nature present in the simulation. One very important command is the *pair_style* because it allows the selection of the models used to calculate the interaction between particles. The available models for this purpose are described in Section 4.2.2.

Run the Simulation

The last phase in the input script preparation is the list of commands to run the simulation. The user should not only specify, in the correct order, which variables are going to be executed, from particle insertion to geometry movement, but also when they should stop. Additionally, right before the running commands, the user should indicate how frequent and in which format it should be stored, otherwise there will be no data output.

4.2.2 Available Models

LIGGGHTS offers a variety of models to calculate the forces exerted by the particles on each other, or interactions with the geometry. In this section, only the ones more adequate for the powder bed simulation, according to what was mentioned in Section 3.4, will be discussed in detail. The software has the ability to calculate forces between two particles when they are in contact ($\mathbf{F}_n$ and $\mathbf{F}_t$) and when they are close enough to interfere with each other ($\mathbf{F}_c$). The general form of a granular interaction force can be written as $\mathbf{F} = \mathbf{F}_n + \mathbf{F}_t + \mathbf{F}_c$, similar to what has been mentioned previously

and the different contributions are calculated according to the selected model.

4.2.2.1 Contact Models

There are two models available for the contact forces calculation, Hertz and Hooke. For both, the coefficients can be linear or non-linear. The contact forces are calculated when the distance between two particles is less than their contact distance or, in other words, when they are touching and compressed against each other. With the Hertz approach, similar to the Hertz-Mindlin from the literature, the normal forces are calculated as [163]:

$$\mathbf{F}_n = k_n \delta n_{ij} - \gamma_n \mathbf{v} n_{ij}, \quad (4.12)$$

where k_n is the elastic constant in the normal direction, δn_{ij} the normal overlap distance of two particles i and j , γ_n the viscoelastic damping constant for normal contact and $\mathbf{v} n_{ij}$ the normal component of the relative velocity of the 2 particles. The tangential forces follow the same approach [163]:

$$\mathbf{F}_t = k_t \delta t_{ij} - \gamma_t \mathbf{v} t_{ij}, \quad (4.13)$$

where all the variables have the same meaning, but are applied for the tangential direction, instead of the normal. The tangential displacement, δt_{ij} , is truncated in order to fulfil $F_t \leq \mu F_n$. The stiffness (k) and damping (γ) coefficients are calculated similar to what has been referred formerly in Section 3.4, but, in addition, are also adapted to accommodate two materials with different properties [163]:

$$k_n = \frac{4}{3} \left(\frac{Y_1}{(1-\nu_1^2)} + \frac{Y_2}{(1-\nu_2^2)} \right) \sqrt{(r_1+r_2)\delta n_{ij}}, \quad (4.14)$$

$$\gamma_n = -2\sqrt{\frac{5}{6}} \frac{\ln e}{\sqrt{\ln^2 e + \pi^2}} \sqrt{\frac{3}{2} k_n (m_1 + m_2)} \geq 0, \quad (4.15)$$

$$k_t = 8 \left(\frac{Y_1}{2(2-\nu_1)(1+\nu_1)} + \frac{Y_2}{2(2-\nu_2)(1+\nu_2)} \right) \sqrt{(r_1+r_2)\delta n_{ij}}, \quad (4.16)$$

$$\gamma_t = -2\sqrt{\frac{5}{6}} \frac{\ln e}{\sqrt{\ln^2 e + \pi^2}} \sqrt{k_t (m_1 + m_2)} \geq 0. \quad (4.17)$$

with Y representing the material Young's modulus, ν the Poisson ration, r the particle radius, e the coefficient of restitution and m the mass.

4.2.2.2 Cohesion Models

Cohesion between particles can exist due to liquid bridge forces, caused by a surface liquid film on the particles, and static forces, also known as van der Waals, that are relevant for small particles. Since the powder in the bed is dry, the first ones can be ignored and only the latter remain. LIGGGHTS offers two simplified Johnson-Kendall-Roberts (SJKR) models that add an additional normal force, strengthening the particles contact, written as [164]:

$$\mathbf{F}_c = kA, \quad (4.18)$$

where A is the contact area between two particles and k is the cohesion energy density. The models are similar, differing only in the way that the area is calculated. The first calculates the area as [164]:

$$A = \frac{\pi (\overline{r_{ij}} - r_i - r_j)(\overline{r_{ij}} + r_i - r_j)(\overline{r_{ij}} - r_i + r_j)(\overline{r_{ij}} + r_i + r_j)}{4 \overline{r_{ij}} \overline{r_{ij}}}, \quad (4.19)$$

with $\overline{r_{ij}}$ being the distance between the particle centres, whereas the second model considers the area to be described as [165]:

$$A = 4\pi \delta n_{ij} (r_i + r_j). \quad (4.20)$$

4.2.2.3 Rolling Friction Models

The rolling friction models add an additional torque contribution. Only two major models are available, the constant directional torque (CDT) and the elastic-plastic spring-dashpot (EPSD), that contains three variations with minor adjustments. The CDT model is based on a publication [166] that describes the rolling friction similar to what was already done, but adapts it, so its compatible with the rest of the code. It is given as [167]:

$$\mathbf{T}_{rf} = \frac{\mu k_n \delta_n \omega_r}{\|\omega_r\| (r_i + r_j)}, \quad (4.21)$$

where ω_r is the projection of the angular velocity ω in the shear plane, with $\omega = \omega_i - \omega_j$.

CHAPTER 5 Computational Model Setup

The main objective of the work, as previously stated, is to develop and assess a model capable of simulating the SLS process and employ it to evaluate the influence of the most relevant parameters. Because each process has a unique setup that heavily depends on the machine, material and part being produced, an in-house process, in a EOS P 396 laser-sintering machine, with a polymeric material, PA2200, will be the reference for this work.

5.1 Geometry

The first step towards preparing the simulation is to build the geometry, in this case, the powder bed, that will be incorporated the simulation domain, later. For the detailed analysis of the various process parameters influence on the sintering evolution, the scale of the problem must be at the particle length and the powder distribution should be as realistic as possible, so that the final results are representative of reality. To reach the indicated standards, LIGGGHTS, a DEM particle simulation software, which was presented in Section 4.2, was used. The main objective of the LIGGGHTS simulation is to obtain a representative section of the powder bed and then generate a computational mesh that will be used later with the CFD software. Performing a simulation of the formation of an entire powder bed would be very time-consuming given the large number of powder particles present in it. Even a single layer would be too large considering that a small representative section is enough to accomplish the objectives. Thus, only a portion of the bed was simulated during the deposition of one layer. The dimensions of this section were selected to accommodate, in thickness, approximately two layers of material, and a surface area that allows the crossing of two consecutive laser scans, which has a fixed laser spot diameter of $473.4\text{ }\mu\text{m}$. Being a meshless method based software, the output file does not contain the particles themselves, but instead a set of data that allows their visualisation, alongside information about their properties over time. For this case, only the particles indices, radius

and position were stored and the visualisation was performed with Paraview.

For the simulation, two geometries, a box and a blade, that are displayed, together with their dimensions, in Figure 5.1.a, were created using a CAD software. Both act as walls, which means that particles collide with them without getting through. The box has a deeper section that can be viewed as a smaller box under the larger one, where the particles will fall, simulating the beginning of the deposition of one layer. This smaller box will contain the representative section of the powder bed. The first step in the simulation is the particles insertion. To ensure that the smaller box is totally filled, the selected amount of particles was large enough so that when the blade moves past it, it still drags a significant amount of powder. In this case, the amount of particles is given by mass and the selected value that fulfils these requirements (without inserting an exaggerated large amount of particles) was 0.115 g. The insertion phase lasts for two seconds and takes place over a area in the far end of the larger box (Figure 5.1.b). It is then followed by the blade movement, that moves at a constant speed in the x direction. Before the inserted powder reaches the smaller box, it has to be dragged over a long flat section that was purposely made in such way, not only to accommodate the particles insertion, but also to assure a more realistic powder distribution because, this way, the particles are packed by the blade movement and their "flow" is more developed before falling into the hole (Figure 5.1.c). Once past the smaller box, the blade will keep moving, dragging the remaining particles past the boundary, outside the simulation domain, deleting them (Figure 5.1.d). At the end, only the particles inside the smaller box will be used for the mesh generation.

The particle interaction models for the powder bed simulation, which are described in Section 4.2, were selected by comparing the models available in the software with the literature on the topic. The software also requires the input of various material properties that are indicated on Table 5.1 [168]. The powder particle size distribution was also taken into account. In LIGGGHTS, each individual particle size has to be specified with its corresponding percentage in mass or quantity. Because of the impossibility to consider an infinite number of particle diameters, or the impracticality of specifying a large amount of them, nine different particles sizes, centred on the highest percentages, starting at 35 μm of diameter and increasing by 5 μm , until the maximum diameter of 75 μm was reached, were defined. Each individual size was represented alongside its respective percentage, in order to approximate the real material distribution that is illustrated in Figure 5.2 [169]. Lastly, for simplification purposes, and also due to the impossibility of manually defining a unique shape for each particle, they were considered to be perfectly spherical, as commonly done in similar studies [47].

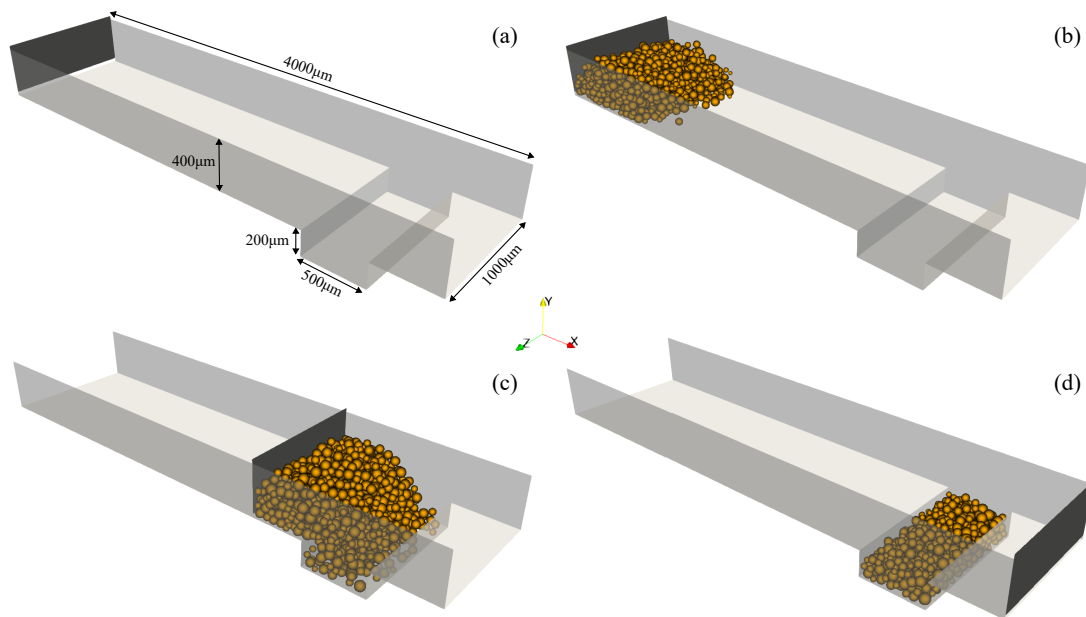


Figure 5.1: Geometry dimensions and various stages of the simulation. Initial time (a), end of particle insertion (b), particles falling into the representative section (c) and end of the simulation (d).

Table 5.1: Polymer powder properties for the simulation in LIGGGHTS.

Parameter	Value
Material Density	1000 kg/m ³
Young's Modulus	2.3x10 ⁷ Pa
Poisson's Ratio	0.4
Coloumb's Friction Coefficient	0.5
Surface Energy	0.1 mJ/m ²

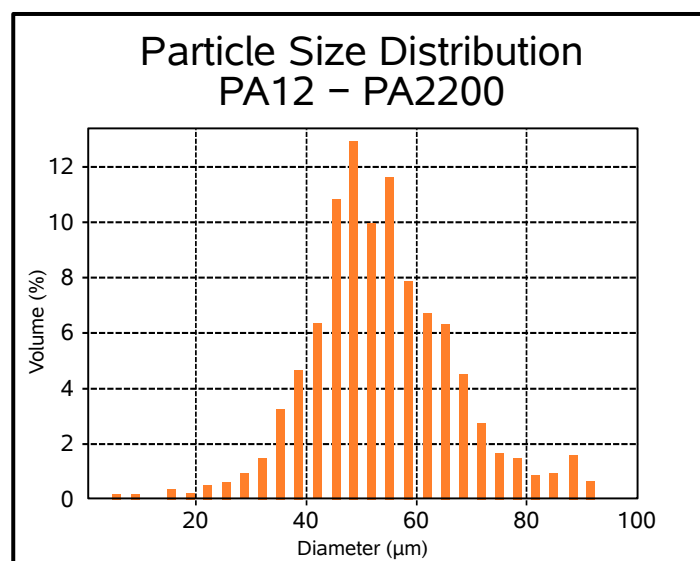


Figure 5.2: Particle size distribution of the selected material for the simulation.

Finally, to validate the results, the bulk density of the simulated representative section was calculated using Paraview. The obtained value was 0.43 g/cm^3 , which is satisfactorily comparable to the material data sheet value of 0.45 g/cm^3 [170].

5.2 Computational Mesh

The representative section of the powder bed simulated using LIGGGHTS needs to be converted into a computational mesh before it can be used by the CFD software. Multiple approaches can be employed for that purpose, but, considering the large number of particles and consequent complexity, some could reveal themselves too complicated or time-consuming, whereas the following approach is simple and practical.

Using OpenFOAM tools, a meshed box with dimensions of $500 \times 1000 \times 230 \text{ }\mu\text{m}$ (slightly taller to accommodate particles that exceeded the top "limits" of the box) was generated using *blockMesh* [171]. Then, the particles in the last time step of the LIGGGHTS simulation needed to be converted into a STL file so they can be used for the mesh generation step. Since the particles are perfectly round, a spherical glyph, that scales with the radius, was created around each particle centre point in Paraview, allowing the simulation data to be converted into a geometry file, in STL format. Finally, with the *setFields* utility [172] from OpenFOAM, the STL file was inserted into the meshed box and the cells that intersected it were defined as solid. By using *blockMesh*, a fully orthogonal mesh with equal sized cells was obtained, while each particle and atmosphere regions are properly set.

When creating a computational mesh, it is important to balance the accuracy with the simulation time, since both will increase with the cells number. For this specific case, the limiting factor are the smaller particles that require a higher resolution (smaller cells) to be adequately represented. Four different refinement levels were tested, starting with the coarsest mesh, that has one cell per $8 \text{ }\mu\text{m}$, and then doubling the number of cells (when possible) in each direction for the next refinement levels, as shown in Table 5.2.

The Coarse mesh (Figure 5.3.a) is clearly inadequate since the geometry is not properly represented. The resolution is so low that the particles barely resemble a sphere, with the smaller ones fitting inside four cell sided cubes. The Medium mesh (Figure 5.3.b), with double the refinement level, already provides a good geometry representation, with well defined spheres and an acceptable definition for the smaller particles. For preliminary simulations, where the main goal is to quickly

Table 5.2: Number of cells for the different levels of mesh refinement.

Name	Cells x-direction	Cells y-direction	Cells z-direction	Total Cells
Coarse	63	29	125	228 375
Medium	125	58	250	1 812 500
Fine	250	115	500	14 375 000
Extra Fine	300	138	600	24 840 000

test some parameters, this mesh is sufficient. For more detailed studies, however, the Fine mesh (Figure 5.3.c) is significantly more adequate. Despite the large number of cells, which will increase the computational cost, the geometry is remarkably well defined, with the particles looking almost spherical. A good refinement level is always desirable since it greatly reduces the error associated with the simulation. Moreover, there will be movement in the liquid phase, caused by surface tension forces, that is expected to be substantially better observed with this mesh. Despite the satisfactory results, an additional refinement was tried. Increasing the refinement further than this is very challenging in terms of computational power since a large amount of memory is required. Due to memory limitations, this time, the increase could not be doubled and, instead, using the available hardware, an increase in 20% of cells in each direction was tested (Figure 5.3.d). As expected, the particles are even closer to their original shape in the STL file, however, considering that the refinement level obtained in the previous attempt was already sufficient to properly represent the geometry and that the Extra Fine mesh has ten million more cells, it was discarded for the sake of computational time. Among the four meshes, the Fine mesh, with one cell per two micrometers and a total of around fourteen million cells, was the selected to perform the studies.

The approach for selecting the mesh is only based on the balance between their geometry representation quality and the number of cells, which is not totally correct, since various simulations with each mesh should have been performed to assess the refinement level influence on the results. However, due to time limitations, such approach was not possible and the next best option was employed.

5.3 Material Properties

The selected OpenFOAM solver, contrary to other popular solvers, considers each state of the material as a separate phase and requires the specification of its properties separately. This translates

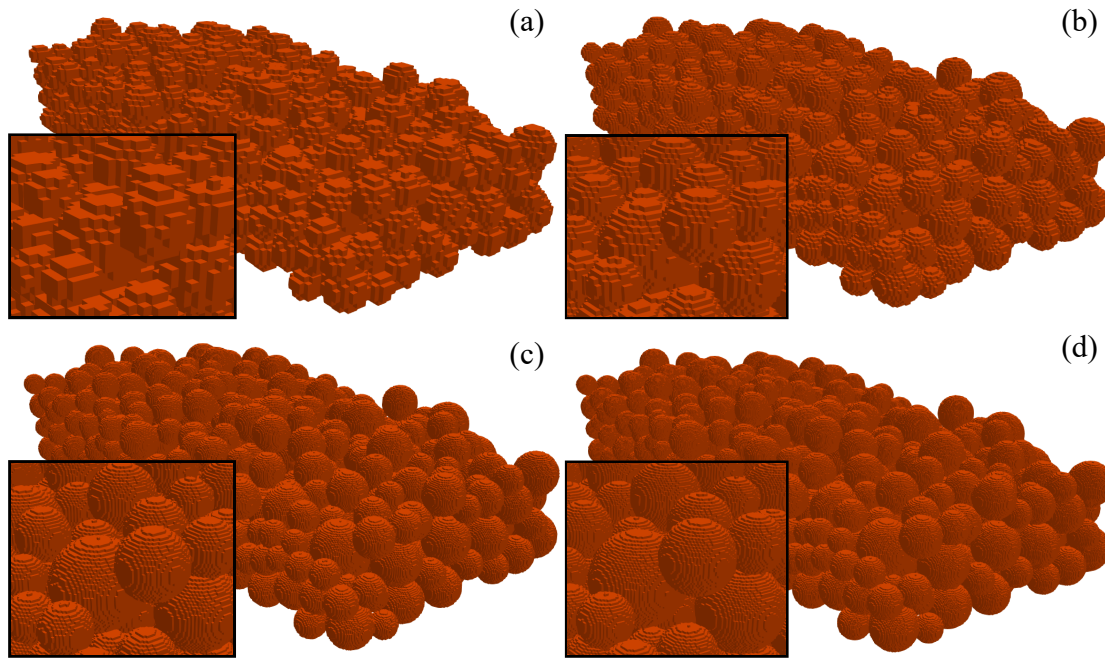


Figure 5.3: Visualisation of the different mesh refinement levels. Coarse mesh (a), Medium mesh (b), Fine mesh (c) and Extra Fine mesh (d).

into some properties, such as viscosity, only being required for one of the phases, in this case, the liquid one. For this specific case, a total of three phase files should be provided: *alpha.solid*, for the initial solid polymer, *alpha.liquid*, for the polymer in liquid state and *alpha.air*, for the surrounding air present in the chamber.

5.3.1 Polymer

The material utilized in the process used for comparison purposes is a widely used polyamide for SLS applications, PA12 - PA 2200, produced by EOS [173]. According to the manufacturer, this PA12 is a high-performance equivalent to well regarded materials in injection moulding, such as ABS or PA6, capable of producing equally strong, flexible and durable parts.

Accurately defining each property for polymeric materials is challenging because of their intrinsically complex behaviours. Most properties, in order to be accurately determined, require the replication of the SLS process conditions that are hard to achieve, or obtained through unconventional characterization methods, which leads to less adequate information available. Taking the viscosity as a first example, the test conditions must be as close as possible to null shear rate to capture the real value without the shear thinning influence, which requires specific rheometers. Another example is the melting point whose values are obtained through DSC tests, generally at a constant heating rate.

However, in the real process, the material is only going to heat at such rates in the pre-heating phase, where no melting occurs. After that, it heats much faster by action of the laser. This is a less accurate way to determine the desired properties, because the rate at which polymers heat can change their melting point and consequently its enthalpy of fusion. Moreover, polymer properties heavily depend on the surrounding conditions, namely the temperature. As already stated, the increase in temperature during the process causes the material to age, a phenomena that will change its properties. Using the viscosity as an example again, even if the powder bed is considered to contain only virgin material, by the time it reaches the pre-heating temperature, due to ageing, the viscosity will no longer be the one initially defined. Similar to these examples, many other properties are challenging to obtain due to suchlike reasons, thus some simplifications and assumptions need to be considered. A common one is to assume temperature independent properties. Although the solver allows temperature dependent properties, no adequate information was found that allowed such definition for several parameters. This should not present itself as a large hindrance since that, although there is a large temperature gradient after the scan, the material will cool down to temperatures closer to the initial one relatively fast [174]. Between the list of parameters that the solver can work with, the useful ones for the simulation are the density, specific heat, thermal conductivity, viscosity, surface tension, melting point, complex index of refraction and coefficient of absorption for the laser. These parameters are indicated in Table 5.3. Starting with the density, the material datasheet only provides information on the bulk powder bed and sintered parts value, with no actual values for the density of the material itself. Therefore, a general value for PA12 of 1000 kg/m^3 was selected. The thermal conductivity was provided by the in-house process operators and the surface tension [102], absorption coefficient [47] and viscosity [110] values were taken from the literature, from articles that considered the SLS process conditions. The latter contains two values, the lower corresponds to the virgin material, and the higher, due to ageing, to the processed one. The two components of the complex index of refraction are the refractive index, with the value 1.6 [175], and the imaginary part, k . Unfortunately, no information was found for the latter component, however, it can be related to the absorption coefficient as $k = \alpha \lambda / 4\pi$ [176], giving k the value of 0.011.

All the aforementioned properties were defined as constant, mainly due to the lack of information to specify them otherwise. The two remaining parameters, the specific heat and the melting point, require a different treatment for various reasons. One of them, the solver does not take into account the enthalpy of fusion, which would help into more accurately accounting the total energy required for phase change. Fortunately, in-house tests were performed on the material that allowed the determination of

Table 5.3: Some of the required polymer properties for the computational studies.

Property	Value	Units
Density	1000	kg/m ³
Thermal Conductivity	0.2	W/m K
Viscosity (at 474k)	390/5095	Pa/s
Surface Tension	0.035	N/m
Absorption Coefficient	1.3×10^4	m ⁻¹
Complex Index of Refraction	$1.6 + i0.011$	—

the specific heat as function of the temperature, which is expected to greatly increase the accuracy of the simulation. Within the temperature range of interest, the values were introduced in the material properties dictionaries in the form of a table. Additionally, not considering the enthalpy of fusion brings an additional challenge for selecting the melting point. Polymers do not have a well defined melting point, but instead, melt over a range of temperatures. Lamentably, the solver does not consider such behaviour and the material will change phase when it reaches the transition temperature. Although the total energy is accounted for with the temperature dependent specific heat, it is still necessary to define a temperature for phase change. In reality, process operators tend to consider the beginning of the melting range, also known as onset of melting, as the melting point that, for this material, is 449.15 K. Doing that for the simulation is inaccurate because it would be largely over predicting the amount of liquid phase, since it would consider as fully liquid any solid cell above that temperature. Similarly, on the other end, only considering the melting point at the end of the melting range would, much likely, promote an under prediction, especially considering that it is around 469 K [177]. Due to these reasons, the selected phase transition temperature is somewhere in between those two, at the peak energy point during the DSC test, commonly referred to as simply the melting temperature. According to the literature, the melting point for fresh PA12 is at 459.75 K and it suffers a slight increase after being used, with a mid point of 460.65 K [175]. Another study, this time for the same PA2200 used in the process being simulated, exhibits a melting point of 461.75 K [177]. Despite the first study providing various temperatures depending on the material use, because there is a very small difference between all of them, the selected one was from the latter study.

Although describing in Section 3.1 the different approaches for modelling the material crystallization, such phenomena was not considered. In fact, once the material liquefies, it will stay in that state throughout the entire simulation. That is because the selected domain is but a representative section that, considering the simulation time and the sintering window, will never reach temperatures

low enough to solidify. Besides that, the main objective of the work is to evaluate the parameters influence on the particles melting and coalescence, which denotes the crystallization as irrelevant.

5.3.2 Chamber Atmosphere

The chamber is filled with an inert gas, usually nitrogen, in order to avoid degradation reactions, such as oxidation. Even though a significant amount of information was found regarding the temperature dependency of the nitrogen properties, they were all defined as constant to simplify the model and alleviate the calculations. Besides that, the material at study is the polymer so, as long as the gas properties are somewhat correct, it should not drastically influence the results. The values for the density [178], thermal conductivity [179], specific heat [180] and viscosity [181], for temperatures within the process range, were all obtained from well-known databases. For the absorption coefficient, no information was found regarding its value for the employed laser, however, a study for other gases, with a CO₂ laser beam at a close wavelength value, showed that the absorption coefficient for gases is much smaller and almost negligible [182]. Since no study on the process mentions the interaction of the laser with the air, it was assumed that it was insignificant, therefore a small value was selected. The gas properties are displayed in Table 5.4.

Table 5.4: Nitrogen properties employed in the computational studies.

Property	Value	Units
Density	0.676	kg/m ³
Thermal Conductivity	3.887×10^{-2}	W/m K
Specific Heat	1049	J/kg K
Viscosity	2.6×10^{-7}	Pa/s
Absorption Coefficient	1	m ⁻¹

5.4 Model Parameter Studies

The proposed solver for the CFD simulation is extremely complex and contains a variety of parameters for tuning the models that are, most of the times, case dependant and, therefore, not available in the literature, especially numerical ones that have no physical meaning. It is necessary to evaluate these parameters influence so one can obtain results that are comparable to those of the real process to assure that there is physical meaning behind what is being simulated. Only after that is it

possible to assess the process parameters influence.

5.4.1 Surface Tension Studies

As already stated in Section 2.4.3.1, the surface tension is the driving force for the coalescence between particles, which makes it extremely important for the process dynamics. Such crucial mechanism has to be accounted for in the model and its behaviour needs to be studied before advancing with more complex simulations. To test the model, two spheres with 50 μm of diameter (the average particle size) were positioned inside a domain where they are not touching anything but themselves, as shown in Figure 5.4. To isolate the studies, all optional models are disabled and the spheres already start in a liquid state at a uniform and constant temperature. Because surface tension is a force opposed by the viscosity of the material, while keeping it constant at a value of 0.035 N/m, two different viscosities were employed in distinct tests, 390 and 5095 Pa·s. The values are, respectively, from the virgin and used material.

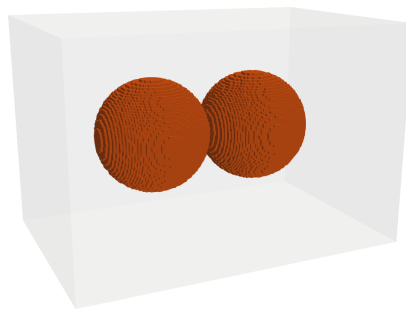


Figure 5.4: Base case geometry for the surface tension studies.

Virgin Polymer

The results from the tests with the virgin material, illustrated in Figure 5.5, show a complete coalescence between the two particles after five seconds, which, considering that the building process lasts much longer, is a fast consolidation.

Unfortunately, no information was found regarding the sintering time between two particles that allowed for a comparison of the obtained results, however, a study on the sintering evolution between two particles of PA2200 by slowly increasing their temperature is illustrated on Figure 5.6 [183]. Despite the absence of a time scale, it is possible to analyse and compare the particles shape and the neck that they form. Figure 5.6.a shows the particles forming a very small neck, in a stage slightly

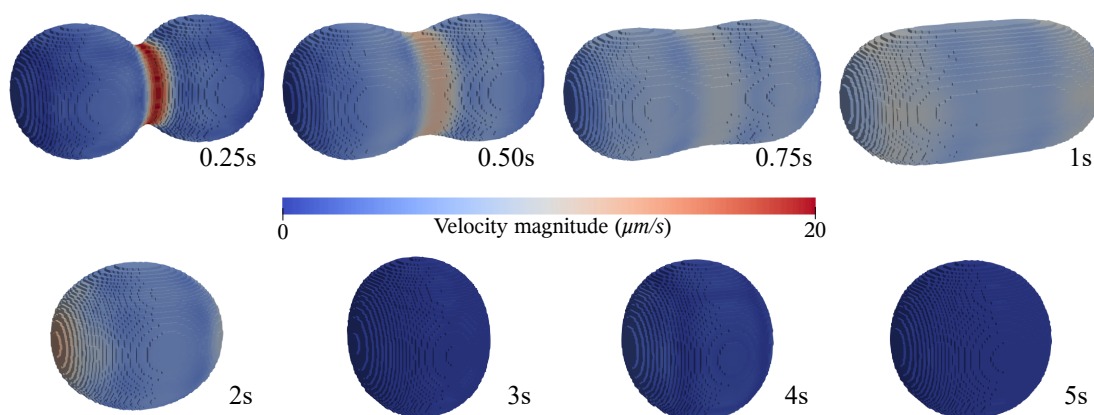


Figure 5.5: Surface tensions studies with virgin material.

before what is visible after 0.25s on the simulation. At Figure 5.6.b, the neck is further developed and the shape similar to the results at 0.5s. Lastly, in Figure 5.6.c, the two particles are now a single one with an oval shape that resembles the results at 2s.

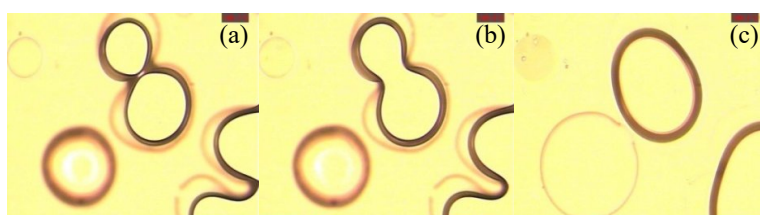


Figure 5.6: Hot stage microscopy of PA12 - PA2200 (adapted from [183]).

Used Polymer

The tests with the used material (Figure 5.7) differ significantly from the previous ones. The used material viscosity is more than ten times larger, which highly hinders the movement of the liquid phase. For these results, a different time scale had to be considered, since it took three seconds for the neck formation to be similar of just a quarter of a second with the virgin material. In this case, the much larger viscosity does not allow for a quick development of the neck and, instead, the particles coalesce partially by attracting themselves.

Mixed Polymer

As previously noted, the material will suffer alterations in its properties, namely an increase in viscosity, due to exposure to high temperatures. There is usually a mix between the used powder and

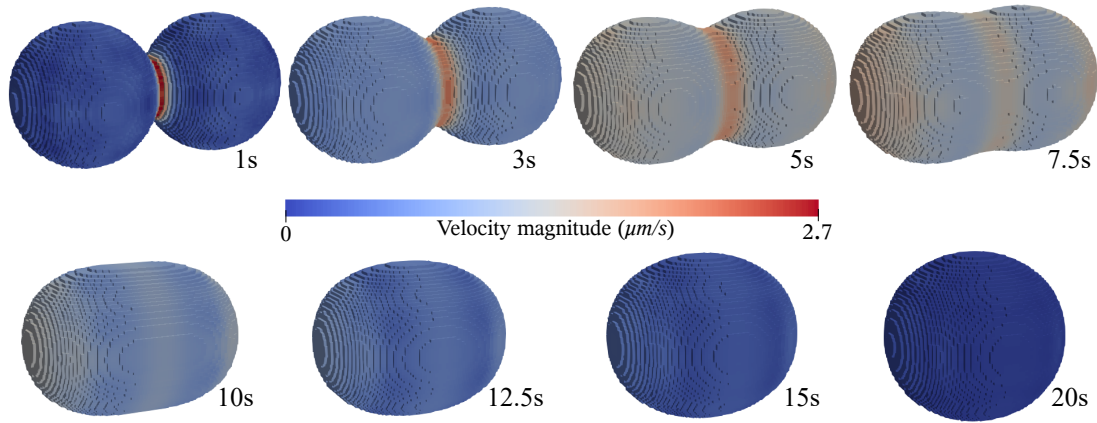


Figure 5.7: Surface tensions studies with used material.

the virgin one in an attempt to diminish the negative effects of ageing. In reality, the powder bed would contain a percentage of each type of particles, virgin and used, that have distinct viscosity levels. For an appropriate case setup, this would require two distinct liquid phases with their respective properties. Unfortunately, the solver fails to consider the surface tension interaction between two different liquid phases and the results are incorrect. In Figure 5.8, two particles of distinct liquid phases, but with identical properties, are positioned in a similar way as for the previous tests. Considering that the imposed viscosity is that of the virgin material, the results should be similar to the ones presented in Figure 5.5, however, as one can clearly observe, they are totally different.

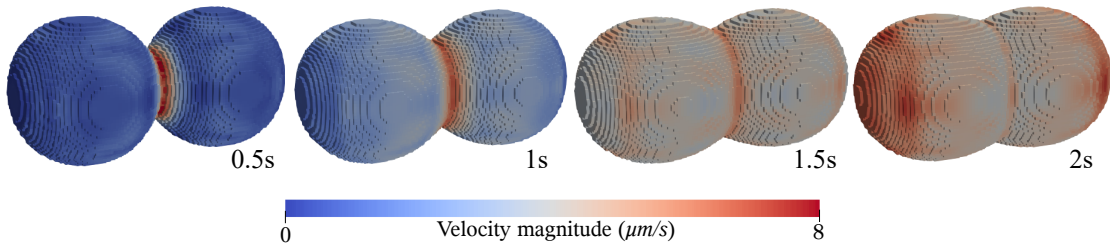


Figure 5.8: Surface tension studies with distinct phases, but with identical properties (2 spheres).

To further prove this incorrect behaviour, another test with four particles, two of each liquid phase, but, again, with identical properties, was performed. The results, shown in Figure 5.9, clearly prove that between the same phase, the evolution is as expected, however, between different phases it is not.

Due to the impossibility of adapting the code to fit the specified needs, the material properties were considered, for simplification, as a pure mixture of virgin and used material, with an average viscosity of 2742.5 Pa·s. The coalescence development with this assumption is shown in Figure 5.10. As expected, the sintering progression falls somewhere in between the virgin and used material cases, stabilizing after twelve seconds.

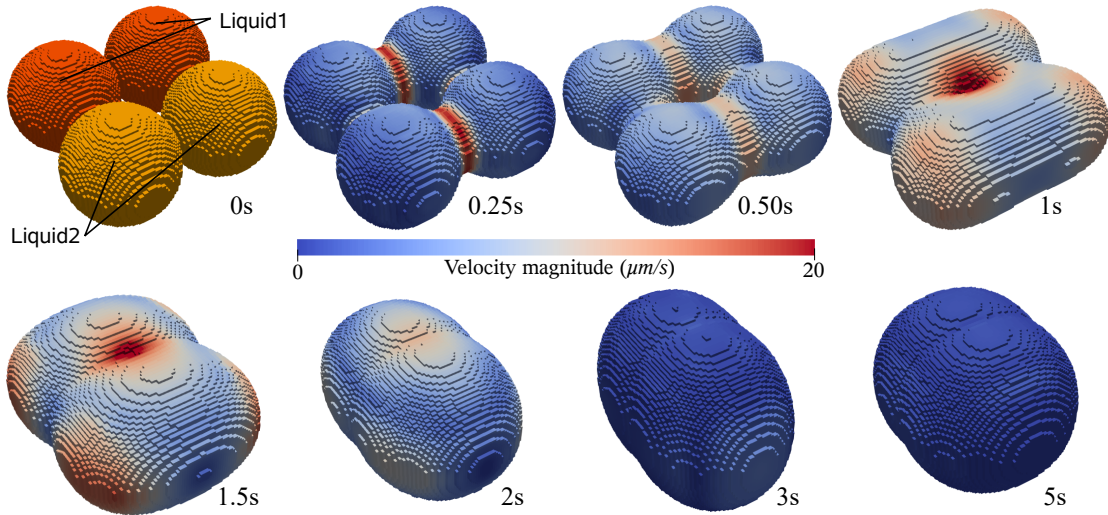


Figure 5.9: Surface tension studies with distinct phases, but with identical properties (4 spheres).

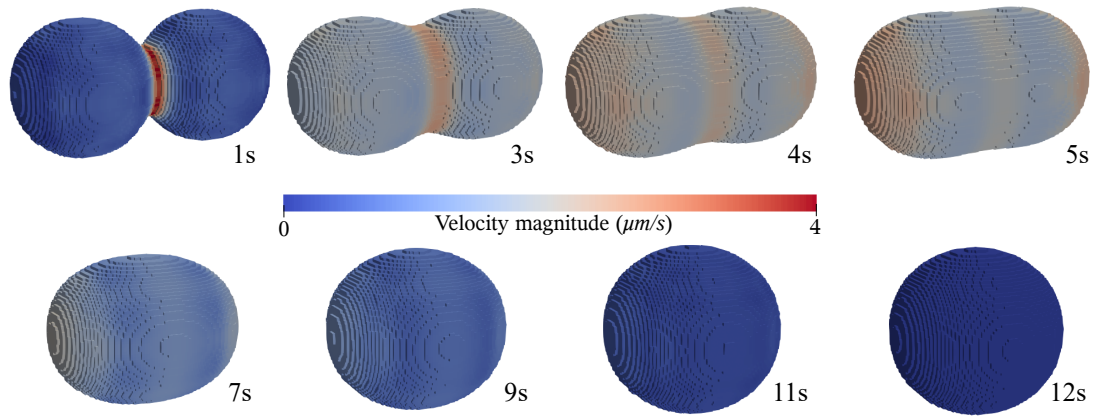


Figure 5.10: Surface tension studies with mixed material properties.

5.4.2 Voller-Prakash Model Studies

For the accuracy of the simulation, it is important that the solid phase stays static. The problem, however, is that the solver considers that the solid phase can be dragged by a moving liquid phase as if it was also a liquid with null viscosity. Considering the problem to be studied, the liquid phase will move due to surface tension forces and, if a solid particle's shape is affected by that movement, the results will be highly unrealistic. The Voller-Prakash model, explained in detail in Section 4.1.2.1, was originally developed to describe with more accuracy the velocity of a material during phase change, where it is in a state in between solid and liquid. Despite that application, the model also works for fixing in space a solid when in contact with a moving liquid. The mentioned problem is illustrated in Figure 5.11, where the previously two spheres (Figure 5.4) are now cut in half and placed on a solid base. Here it is visible that the solid blocks are moving due to the forces exerted by the liquid phase. These results are not

realistic, hence the need to fix it. The implementation of the Voller-Prakash model in OpenFOAM comes with a constant whose increase is directly proportional to the intensity of the effect. One could select a ridiculously large value that would totally fix the solid phase, however, that could result in numerical instabilities. Instead, to avoid these issues, tests with different constant values were performed until a minimum value, that assured the expected behaviour, was found. Among the various tests, three were selected as an illustration of the models purpose.

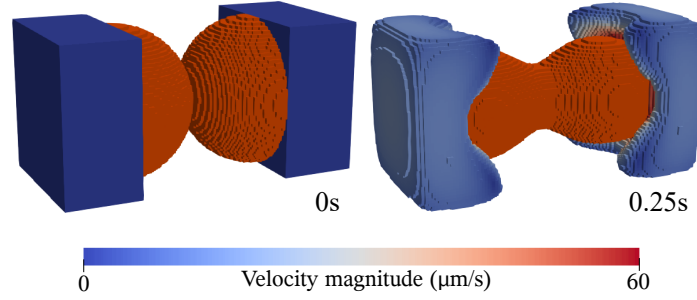


Figure 5.11: Unwanted movement of the solid phase due to the absence of the Voller-Prakash model contribution.

The first test illustrated has a value of 10^5 for the model constant which, without any comparison, might seem like a large value for a first test. However, looking at the results presented in Figure 5.12, it is obvious that this value is still too low, not only because there is still a large amount of movement in the solid phase, but because the movement is almost identical to the example without the model contribution.

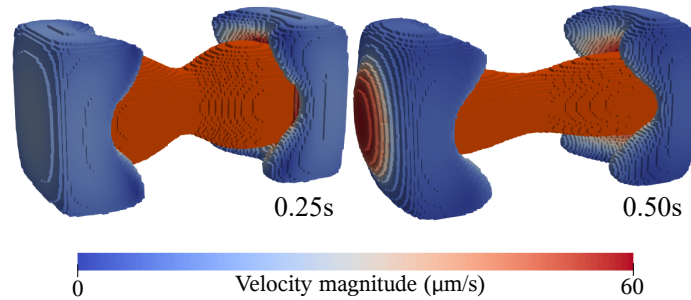


Figure 5.12: Studies on the velocity of the solid phase with Voller-Prakash model's constant of 10^5 .

Increasing the constant value to 10^{10} greatly reduces the solid blocks movement, as Figure 5.13 shows. Nonetheless, there is still a significant amount of distortion that will tend to get worse considering the cells velocity magnitude.

The minimum value considered acceptable for the constant was 10^{15} , whose results are shown in Figure 5.14. For this case, the solid phase has no visible deformation and only a small amount of the

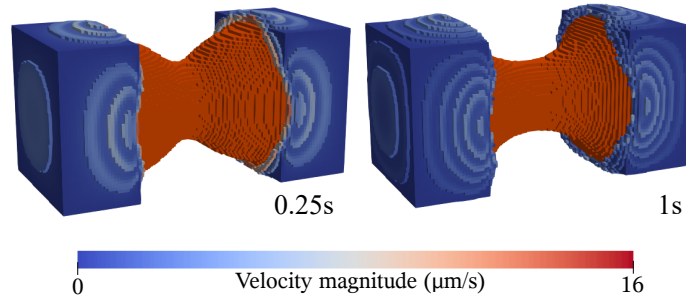


Figure 5.13: Studies on the velocity of the solid phase with Voller-Prakash model's constant of 10^{10} .

corresponding cells present non-null velocity (probably because they contain a small liquid fraction) that, itself, is extremely low and can be considered negligible.

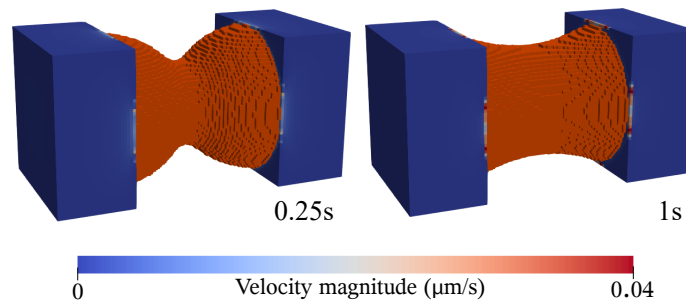


Figure 5.14: Studies on the velocity of the solid phase with Voller-Prakash model's constant of 10^{15} .

5.4.3 Lee Model Studies

The mass transfer during phase change is modelled by the Lee model, which is the only model available in the solver for melting and solidification applications. This empirical model contains a constant that, besides working as a switch to indicate if melting or solidification happens, also functions as a mass transfer intensity indicator. This coefficient is difficult to measure experimentally and its selection is case dependent. From the more detailed explanation of the model in Section 4.1.2.1, some values were highlighted from the literature, ranging from 0.1 to 7.5×10^5 . For smaller scale problems, some authors select even higher numbers [158]. The problem with selecting an inappropriate value is, in a melting case, for example, the temperature of the solid phase might surpass significantly the activation temperature, also known as the melting point, with an insufficient mass phase change rate. In reality, this is almost impossible to achieve because the energy transferred to the material is used to promote its phase change, therefore the solid phase should have its maximum temperature close to its melting point. This is more predominant in applications where the material heats very fast because there is not enough time for melting to occur, hence the need for higher values for the mass transfer

intensity coefficient. In order to study this parameter, two identical solid spheres, similar to the same base case in Figure 5.4, will be scanned by a laser with typical process parameters, for both velocity and power, and then their temperature profile is evaluated as soon as the scan ends. The selection of the coefficient will be based on how fast phase change occurs and how close the temperature of the solid phase is to its melting point at 461.75 K.

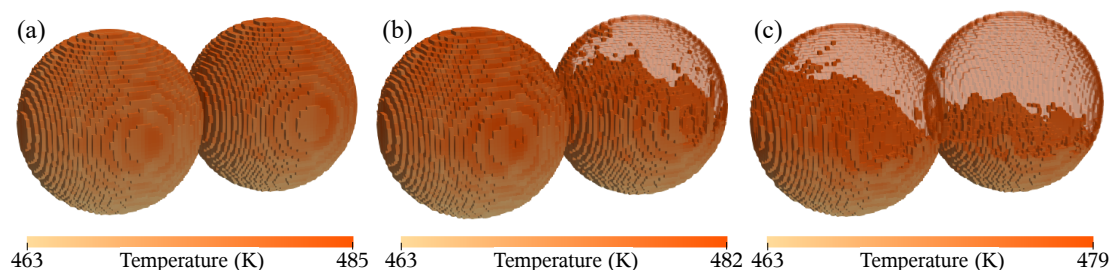


Figure 5.15: Studies on the Lee model mass transfer intensity coefficient with values of 10^5 (a), 5×10^5 (b) and 7.5×10^5 (c).

Figure 5.15 shows the results for three different coefficient values of 10^5 , 5×10^5 and 7.5×10^5 . The first result, shown in Figure 5.15.a, with the lowest coefficient, has a maximum temperature of 23K above the melting point and no phase change has occurred. In Figure 5.15.b, however, a significant portion of the sphere has converted into liquid (displayed as transparent) and the maximum temperature for the solid phase lower by three degrees. Lastly, increasing the coefficient to 7.5×10^5 decreased the maximum temperature by the same small amount as before, but greatly increased the liquid fraction. Despite only showcasing these three results, more studies with different values were performed. Any value below 10^5 , as expected, gives the same results, since no melting occurred. On the other side, although the results with the higher value are still not physically correct, increasing the value further caused numerical instabilities, compromising the simulations. This results, albeit physically incorrect, do not present any concerns for the future simulations because the material will eventually melt. One should note that, at such small scales, the time it takes to scan these two particles is 1.3×10^{-4} seconds. If half the heated zone of the spheres melted after this time, the other half will, most likely, melt very soon. That is also proved by looking at the sphere on the right, that, despite only being scanned a fraction of that time before, has a larger melted zone. Taking into account the slow nature of the sintering process, such small times are considered instantaneous. Nonetheless, if at a later point, during the final simulations, any problem related to this coefficient is found, new tests will be performed to identify a more suitable value.

5.4.4 Laser Studies

The solver makes use of the DTRM to simulate a volumetric heat source. Because it is a ray tracing based model, the user must specify how many rays there are inside the laser domain. Each laser carries energy that will be given to the cell once it passes through it, so it is important to define an adequate amount of rays, otherwise the energy will be improperly distributed. This specific model allows the selection of the number of rays in the radial and angular directions. There are no correct values for these parameters, since they are merely numerical, but a larger number of rays will result in a more balanced accurate distribution. Considering the mesh resolution of one cell per two micrometers and the laser radius of around 237 μm , a total of 119 rays in the radial direction was selected to obtain a ray per cell. This line will repeat itself once every two degrees for a total of 180 times. This selection criterion is similar to others found in the literature for a similar model [47] and increasing it did not exhibit any visible difference, therefore, it was kept at the stated value.

For the reflection model, Figure 5.16 shows a comparison of results with and without the Fresnel reflection model. Looking at the temperature profile for both the middle cross section (figure bottom part) and the top view (figure upper part), one concludes that the model, with the selected parameters, shows minor effects for its contribution. In fact, the maximum achieved temperature with the reflection model was just 2.5 K lower. The literature reports the reflectance of PA2200 to be between 4-6% [184], which indicates that there should not be a major change in the temperature profile. It is still uncertain if the model is adequate for this application but for now, since the increase in computational time by including reflection was significant and the differences were minimal, the model will not be included in the final studies.

Besides that, some other assumptions on the laser behaviour were made for the sake of simplicity. In the real process, the laser comes from a fixed place somewhere in the top of the chamber. This implies that the shape of the laser spot will not always be perfectly circular and that there will be an incident angle. For the simulation, the laser is always assumed to be perpendicular to the top of the representative section, with a perfect circle for the spot shape.

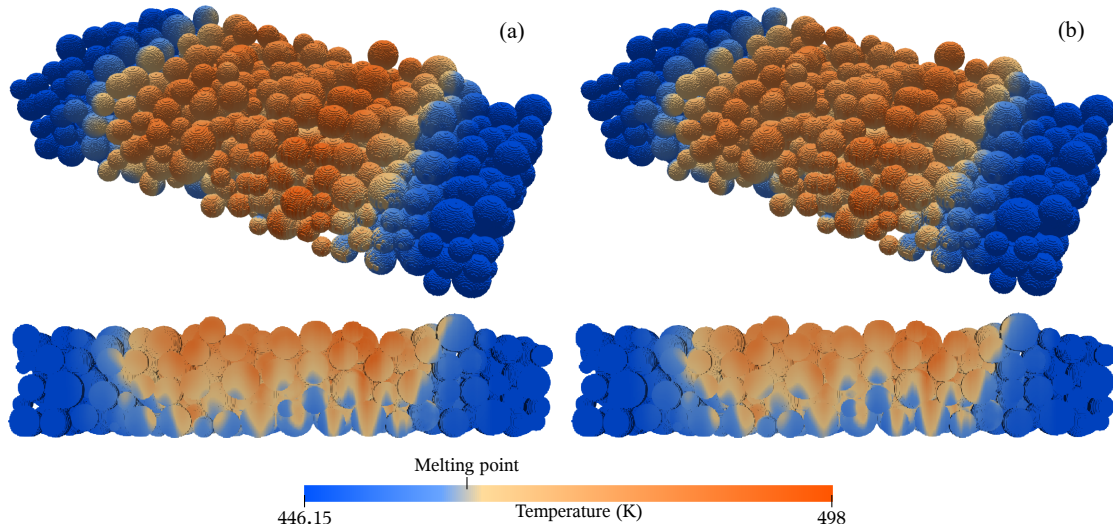


Figure 5.16: Comparison results between not using (a) and using (b) the Fresnel reflection model.

5.5 Initial and Boundary Conditions

OpenFOAM, similar to other CFD software, requires the specification of the initial conditions in order to define a starting point for the simulation. Besides that, the solutions for the boundary problems are also necessary to solve the system of equations. For this specific simulation on the selected solver, the user must specify the initial and boundary conditions for the temperature, pressure, velocity and fraction of each phase.

Temperature

Since the performed studies aim at evaluating the process evolution during and after the laser scan, the temperature conditions are those of the bed after the pre-heating phase. At this stage, as mentioned previously, both the powder and the air are at the same temperature, usually a few degrees below the material melting point. According to the experimental reference data, the initial temperature for the entire domain is 446.15 K. Forcing all the boundaries to maintain this value throughout the simulation would be unrealistic, since it would impose a large difference between the boundary face and the cell value, especially for the regions where the laser passes through. Therefore, the lateral and bottom boundaries were defined with a null gradient condition, which should avoid such large temperature gradients, although considering these boundaries as adiabatic is still not representative of the real process. The top patch, because it is not in contact with the spheres, was kept constantly at the initial temperature, since natural convection is expected to redistribute energy to the large process

chamber and, therefore, the global temperature increment in the air is expected to be negligible.

Velocity

In the beginning of the simulation, the particles are at a solid state and stationary, therefore, a null velocity was imposed in the entire domain. As the process evolves and the liquid fraction is formed, due to surface tension and gravity forces, the liquid phase develops a velocity profile. To assure that no liquid fraction is lost through the boundaries, they can be treated as walls by imposing a null velocity, however, with this approach, the molten particles will stick to the boundaries, which is unrealistic since, in reality, there are no physical walls limiting the section in the powder bed. To prevent that, a null velocity gradient was imposed in the boundaries with the obvious exception of the bottom patch that was treated as a wall, otherwise the entire mass would fall outside the domain due to gravity. By employing these boundary conditions on the lateral and top boundaries, mass exchange with the exterior is possible. Although not entirely realistic, this approach, among the available options, is the most suitable because it does not promote infeasible results as the null velocity does. Moreover, in this specific case, the particles on the periphery of the domain will always be less representative of reality, due to the unavoidable unrealistic boundary conditions, therefore, it is more adequate to select the conditions that do not impact negatively the rest of the domain.

Pressure

The process takes place inside a closed air tight chamber to prevent non-inert gases from contaminating the controlled atmosphere. However, at such a small scale, the representative section is but a small amount of particles surrounded by an atmosphere in a large space. Considering that, and also the fact that the velocity boundary conditions were imposed as a null gradient, the pressure for all the boundaries was set with constant atmospheric value. The initial time is under the same conditions, therefore, the same value was imposed for the internal cells.

Phase Fraction

The absence of inlets in this problem simplifies the boundary conditions for the phase fraction of all phases to a null gradient. The initial conditions that represent the starting phase distribution were defined with the *setFields* utility. This way, the cells in the internal field are represented with

a non-uniform list of scalars where all the cells containing the particles are defined as *alpha.solid* with values of 1 and the remaining cells with *alpha.air* values of 1. The *alpha.liquid* phase is also considered, however not at the initial state.

5.6 Assessment Studies

After generating a computational mesh, defining the properties for each phase, studying the models for the major phenomena, selecting values for their numerical constants and providing the initial and boundary conditions, the first simulations can be performed. However, before directly assessing the parameters influence, one should first compare the process with experimental results to evaluate the solver behaviour and accuracy. Only if the results resemble those of the experimental cases, considering, obviously, that some simplification are being employed and some parameters are taken from external sources, can it be concluded that the developed methodology is adequate to study the process and its parameters influence.

Conveniently, the experimental cases that are going to be used as a reference are from the same in-house process and are available in an article containing information on the process parameters as well as the respective results at a microscopic level [185]. In this article, a complex geometry with various details was produced for dimensional and geometric evaluation. Among those details, there are squared structures with ten millimetres sides and various heights. Because these structures were later analysed in the article, the representative section was assumed to be in the center one of those squares, and the resulting laser path is shown in Figure 5.17. As a note, the only relevant effect of the representative section location is the time between adjacent scans that, in practice, would translate to the energy from the first scan having more time to dissipate before the second scan hits. In these studies, the geometry will be scanned by two adjacent lines and the particles inside the scan area will be analysed.

For the following studies, the material properties, model constants, mesh and simplifications will be the ones stated in the previous sections. The only differing variables between tests will be the process parameters that will be selected according to the study. Three different cases, from the article of reference, with low, medium and high energy parameters, will be used as a base for comparison. A vertical cross section of the scanned part for each case, which will be used later to compare with the simulation results, is illustrated in Figure 5.18.

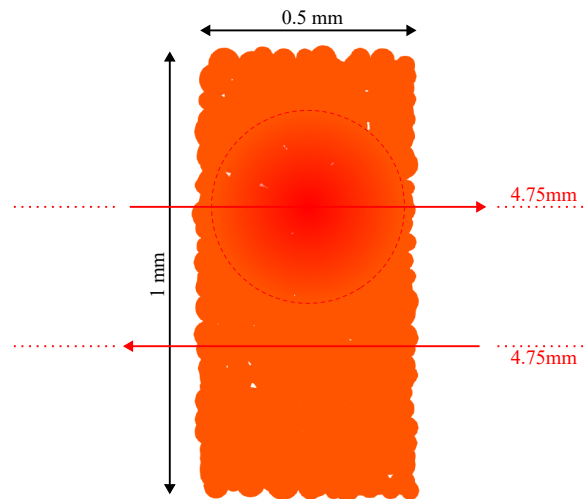


Figure 5.17: Representative section top view and laser path.

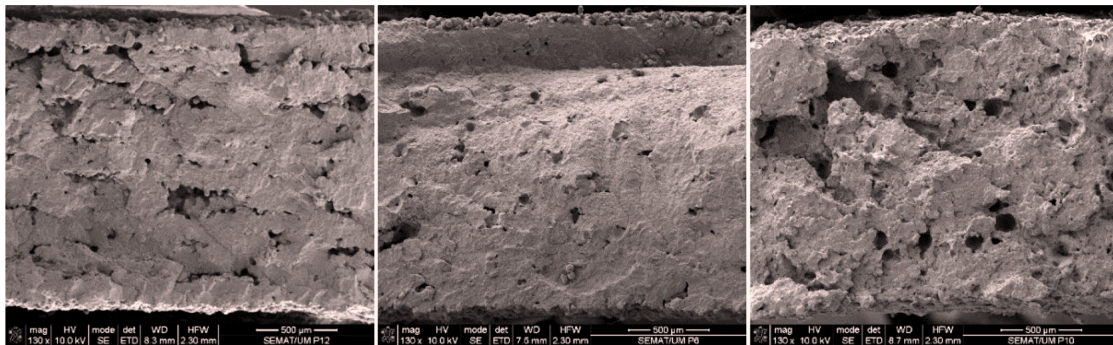


Figure 5.18: Cross section of samples obtained with low (left), medium (middle) and high (right) energy parameters (adapted from [185]).

5.6.1 High Energy Case

The experimental test case with high energy parameters lead to the degradation of material, as it is clearly visible in the right image in Figure 5.18, by the burned aspect of the material and large holes present in the cross section. Unfortunately, the current solver is not equipped with a degradation model, but validation can be performed by comparing the material temperature profile after the scan with the results from the in-house thermogravimetric analysis (TGA), shown in Figure 5.19. The laser scan parameters used for this test case are shown in Table 5.5.

Table 5.5: Laser scan for the high energy case.

Parameter	Value	Units
Power	38.7	W
Scan Speed	3000	mm/s
Hatch Distance	0.3	mm

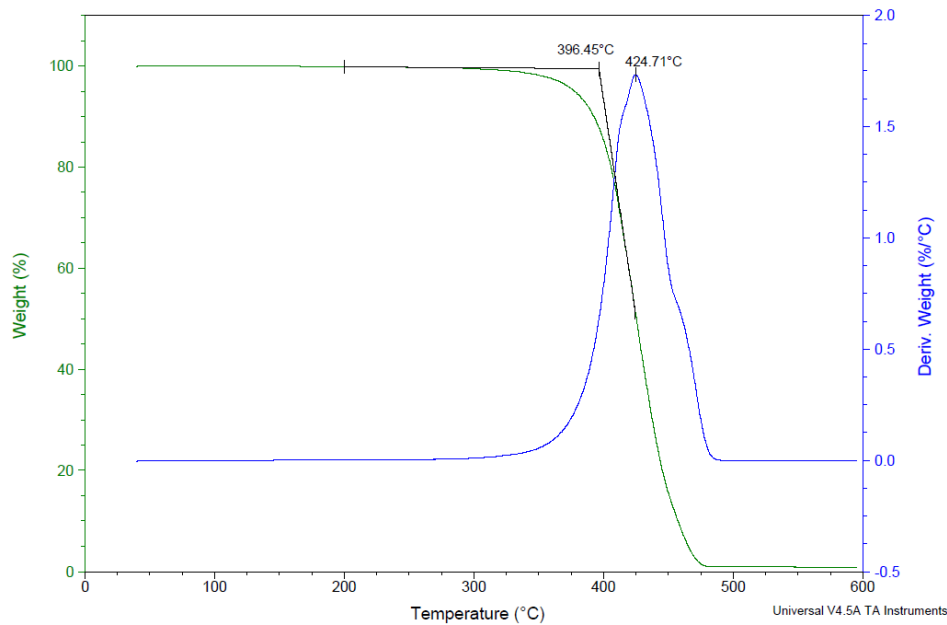


Figure 5.19: TGA of PA2200.

The simulation results, displayed in Figure 5.20, show that, with the selected parameters, there is, indeed, an excessive amount of energy. Considering that the geometry contains approximately two layers of material, the energy transferred to the material is enough to fully melt both immediately. Besides that, looking at the temperature scale, every zone in red, or a reddish tone, is above the temperature for the beginning of degradation of 574.15 K/300°C, that was taken from the TGA results in Figure 5.19, and is associated with the temperature where the degradation curve begins. Degradation seems to be more prominent at the powder bed surface, especially where the two subsequent scans overlap, as visible in Figure 5.20.b. The experimental results do not show major degradation, which indicates that the material did not reach the onset of degradation of 669.6 K and was, most likely, closer to values where the degradation rate was much less accentuated. Based on such comparison, it seems that the temperature profile obtained in the simulation is close to the experimental observations.

5.6.2 Medium Energy Case

As previously discussed in Section 2.4.1.1, despite its inaccuracy, researchers commonly use Drexler's energy density equation (Equation (2.1)) to calculate the energy density provided by the laser. These values are then used, along with their respective experimental results, to determine whether or not more energy is needed. This information is being mentioned again because, unfortunately, the experimental results for the medium energy case do not come with their respective process parameters,

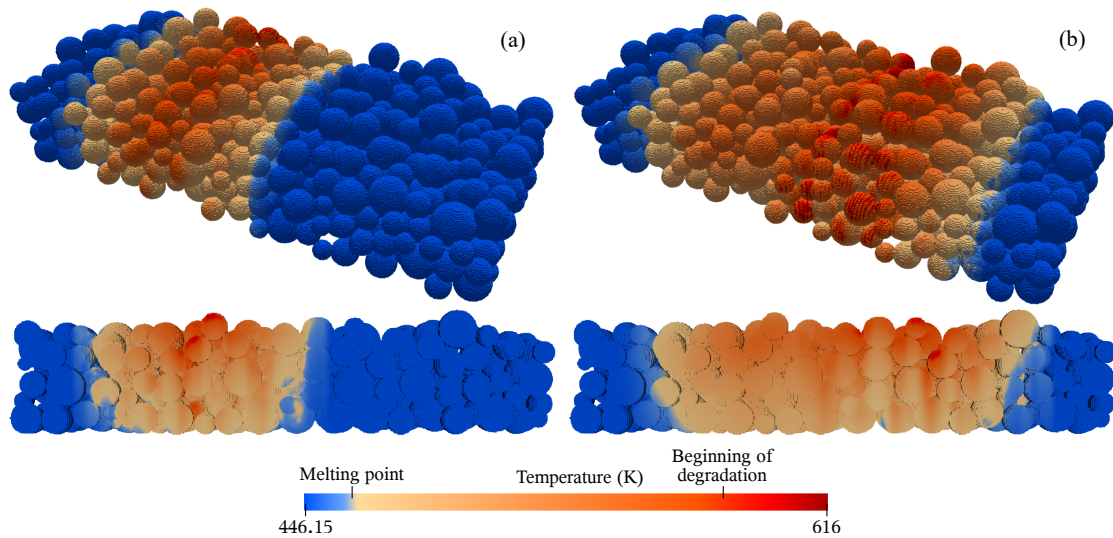


Figure 5.20: Temperature distribution after the first (a) and second (b) laser scans for the high energy case.

but the energy density calculated with the aforementioned equation is known. It is also known that the layer thickness and hatch distance were the same for all test cases so, assuming that the scan speed is also maintained, the laser power can be calculated. The resulting laser scan parameters are indicated in Table 5.6 .

Table 5.6: Laser scan parameters for the medium energy case.

Parameter	Value	Units
Power	30	W
Scan Speed	3000	mm/s
Hatch Distance	0.3	mm

Looking at the simulation results in Figure 5.21, one can conclude that the provided energy is more than enough to fully melt the scanned zone for one layer, with plenty still remaining to reheat the previous one for a good layer adhesion. Compared with the high energy case, by lowering the power by 22.5%, the maximum temperature lowered by 45 K, just a few degrees over the beginning of minor degradation. The experimental results do not display any signs of degradation, only an almost fully dense region with minor porosity from, most likely, powder bed formation defects. This implies that the material achieved high temperatures that promoted fluid flow, by lowering the viscosity, and allowed the particles to coalesce easier. Judging by the impossibility to detect layer separation, the energy provided must also have been enough to reheat the previous layers, which lead to a good layer adhesion. The numerical results, based on the temperature profile after scan, reasonably match the experimental ones.

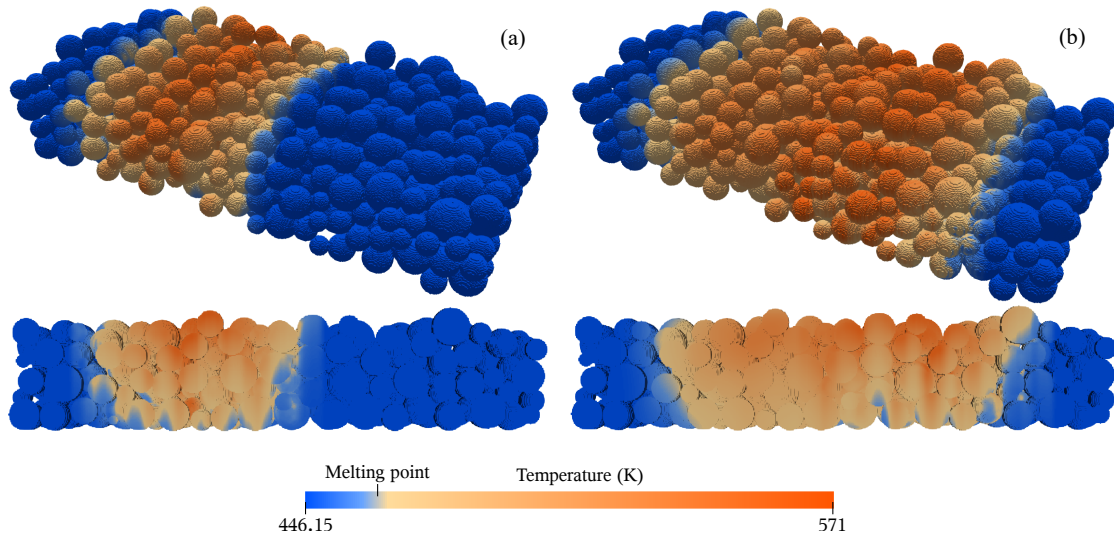


Figure 5.21: Temperature distribution after the first (a) and second (b) scan for the medium energy case.

5.6.3 Low Energy Case

The last case, whose laser scan parameters are indicated in Table 5.7, has a significant decrease in laser power and, consequently, energy density. After analysing the experimental results, one can conclude that the diminishing energy clearly affected the built part since there is poor adhesion between some interlayer sections. Nonetheless, most of the cross section is fully dense and no unmelted particles are visible, which denotes that the lack of coalescence in the defective zones might be related to something else.

Table 5.7: Laser scan parameters for the low energy case.

Parameter	Value	Units
Power	17.1	W
Scan Speed	3000	mm/s
Hatch Distance	0.3	mm

The numerical results for the representative section temperature profile after the laser scan, visible in Figure 5.22, are in agreement with what was mentioned in the previous paragraph. There is, indeed, enough energy to effectively melt one layer and reheat a significant portion of the previous one. However, due to the notable power decrease, the melt depth and overall temperatures are now much lower. Since in this case, contrarily to the previous ones, the energy transferred to the material is insufficient to melt the entire section thickness right after the scan, the simulation was left to run until the remaining particles either melt through conduction, or the overall temperature reaches an

equilibrium.

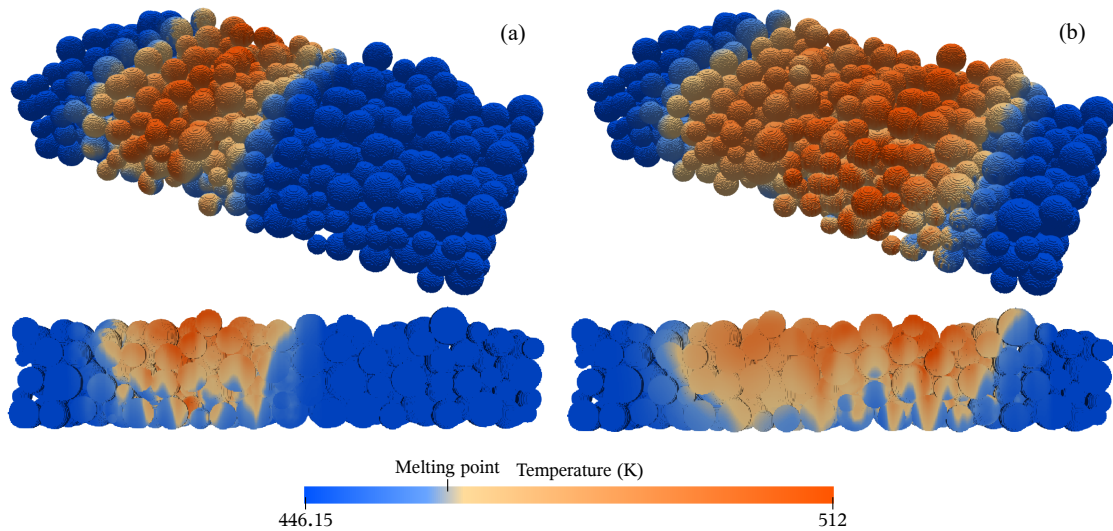


Figure 5.22: Temperature distribution after the first (a) and second (b) laser scan for the low energy case.

After just two seconds, the dissipated heat was enough to melt the bottom of the section, as observed in Figure 5.23. As a note, in reality, the average temperature of the domain would be lower due to natural convection currents that further cool the material beyond the heat dissipation promoted by conduction. These phenomena are generally considered for domains with a continuous media with a heat convection boundary condition at the surface [44], but, for these studies, that alone is insufficient, because the polymer and air are two distinct phases, which results in natural convection inside the domain as well. To consider natural convection within the current model, a temperature dependant density for the air would be necessary, whereas a Boussinesq approximation is also often employed provided that only small temperature gradients exist. However, for the former strategy, a compressible model needs to be considered for a variable density, whereas the current solver assumes the incompressibility condition. On the other side, the latter strategy cannot be considered since high temperature gradients arise in the SLS process. Therefore, the air was defined with a constant density and the only possible consideration for the natural convection was the temperature imposed on the top patch (see Section 5.5).

One could argue that, if the entire section (that represents two layers) is fully melted, poor layer connectivity should not exist, after all, the particles are liquid and will remain in that state until the cooling phase. In the simulation, because the viscosity is set as a constant and has an a value between the virgin and used polymer, that would be the outcome. In reality, however, such simplification do not apply. Starting with the powder mixture, half of the material is guaranteed to be virgin, while the

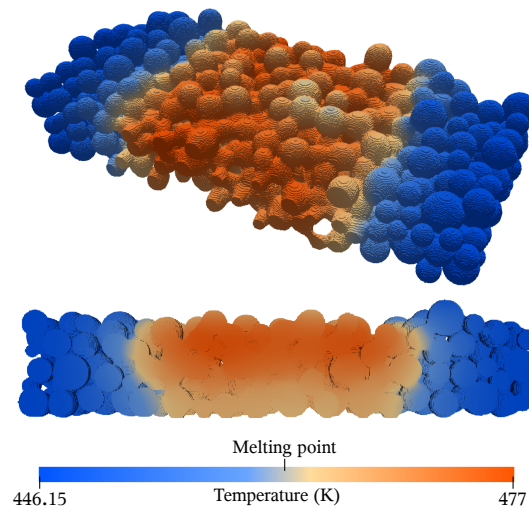


Figure 5.23: Temperature distribution two seconds after the scan for the low energy case.

remaining half is used, which is a very vague definition, since it does not specify how many hours or cycles each portion has. This entails that, among the used particles, different levels of viscosity are possible. Besides that, the surface tension, also set as a constant in the solver, decreases with material use [110], further contributing to a reduced coalescence. Additionally, and most likely the main reason for the poor interlayer coalescence in some regions, the viscosity levels decrease exponential with increasing temperature [109], which means that, although being liquid, particles that receive more energy will coalesce more and faster. In fact, by comparing only the experimental results with low and medium energy, it is safe to assume that both would contain formation defects and particles with high viscosity levels, still, in the medium energy case, the material, because it reaches much higher temperatures that greatly reduce its viscosity, is able to effective coalesce into an almost fully dense part. Taking that into account, when analysing the simulation results, the molten zone, after just three seconds, has a maximum temperature of 474K on the core of the first layer that, coincidentally, corresponds to the temperature at which the viscosities for both the used and virgin material are known. Below and around that zone, the temperatures are considerably lower thus the viscosity will greatly increase. Despite the lack of information on the temperature dependent viscosity and its implementation in the model, the temperature profile on the simulation results, considering what was discussed, present the same behaviour as the experimental results.

5.7 Parameter Influence Studies

During the modelling phase, several simplifications had to be done due to some existing limitations, mainly in time, computational power and lack of appropriate data. Despite that, based on the comparison with the experimental results, the solver proved to be capable of reproducing the SLS process, at least for the temperature profile and temperature evolution. Knowing that the solver is not only behaving in a physically correct way, but also providing results close to the reality, allows the continuation to the next step, the study of parameters influence.

With the comparison tests alone, it was visible what happens when more or less energy is given to the material. Performing more simulations with various energy density levels would not provide much more information on the solver capability or provide additional insights about the process, since the experimental results already provide the extreme energy levels for the employed material. The objective of the following studies is to change some parameters, one at a time, in the direction that would help improve the process by making it faster and/or cheaper, while securing the desired properties. During these analysis, other phenomena, such as dimensional accuracy and sintering evolution, can also be studied. For the base case, the used parameters will be those of the low energy case because, despite not being considered optimal, it was the only one where the entire scanned zone was not fully melted right after the scan. This will, hopefully, allow for a better analysis of the parameters influence, since the sintering depth can also be measured. This section will serve as an introduction to the proposed tests and the respective results and their discussion will be presented in Chapter 6.

Fusion Depth

From the experimental results, both extremes in terms of energy were assessed. That being said, in all the tested cases, the fusion depth was always superior to one layer as a consequence of the high energy needed to lower the material viscosity and avoid the defects seen in the low energy case. It would be interesting to find the lowest energy needed to effectively fuse one layer and reheat just a small portion of the previous one because, as mentioned in Section 2.4.3.4, not all PA12 behave in the same way PA2200 does. PA12 - Orgasol, for example, is much more resistant to ageing and, as a result, the difference in properties, such as viscosity, between virgin and used material, is much less accentuated. For a powder bed that contains material with similar properties, with reasonable viscosity levels, that does not require higher temperatures to lower them for increased coalescence, having a

fusion depth much superior to the thickness of the layer is a waste of energy.

First, to determine the energy needed for the fusion depth of just one layer, the power will be decreased until that objective is achieved and then, using Drexler's equation (Equation (2.1)), the energy density for that power will be calculated. With that value, maintaining the original parameters, the corresponding scan speed will be calculated and both results will be compared. The purpose is to evaluate whether the researcher's common approach of using that equation is adequate and if, independently of the selected parameters, as long as the energy density is the same, so will be the results.

Hatch Distance

The only parameters that was never changed during the experimental results was the hatch distance, so no information is recorded regarding its influence. It is expected that decreasing the distance between scans will concentrate more energy and increasing it will cause the opposite. Because the objective is to adjust the parameters in the direction that will benefit the process, only the latter option will be tested. With the current hatch distance, as the results from the previous section prove, there is no scarcity of energy to evenly heat the material, if anything, where the scans overlap is where some of the maximum temperatures are located. The hatch distance for SLS is, theoretically, limited by the diameter of the laser spot, as it would make no sense to leave a gap of unscanned material between scan line. Its current value is 300 μm and, considering the spot diameter of 473.4 μm , it cannot be increased much more. In this regard, the upper limit for the hatch distance will be tested and its value will equal the laser spot diameter. If this value turns out to be too large, a value between the current hatch distance and the maximum theoretical one will also be tested.

Coalescence

The viscosity is one of the main part quality dictating properties. It is directly related to the degree of coalescence and, based on the experimental and simulation results discussed in the previous section, it can cause severe defects. The current viscosity levels are assumed with a value between the used and virgin material due to the incorrect interaction between distinct liquid phases. Although the viscosity is already being simplified in the model by having its values not depending on the temperature, it would be very interesting to compare the sintering evolution between a powder bed with mixed material and

fully reused one. The real process holds the material at its liquid state for a long time, sometimes hours. Due to the impossibility of running a simulation for that long, a much lower simulation time will be considered.

Dimensional Accuracy

One dimensional defect associated with the process is the lateral increase of parts relative the the scanned area, also known as part growth. The laser has a Gaussian intensity distribution, making it challenging to accurately determine the effective melting area because there is much less energy provided to the the material on the scan spot periphery. The material on these outer zones might melt through conduction but, depending on the total energy, more or less volume will fuse. There is available machine software to compensate for this phenomenon, but it requires prior experimental tests for calibration [186]. The previous cases with the experimental values will be extended until melting stabilizes and then, the liquid fraction in function of the scanned zone will be evaluated.

CHAPTER 6 Results and Discussion

In this section the results for the purposed test cases, described in Section 5.7, will be presented and discussed.

6.1 Fusion Depth

Power Decrease

By decreasing the laser power, as expected, the fusion depth and average temperature of the domain also decreased. The results in Figure 6.1 show that, with a laser power of 10 W, after the scan, the fusion depth is around two thirds of one layer. Judging by the results obtained for the base case, the excess energy present at the top of the layer will eventually dissipate through conduction and melt the remaining of the layer.

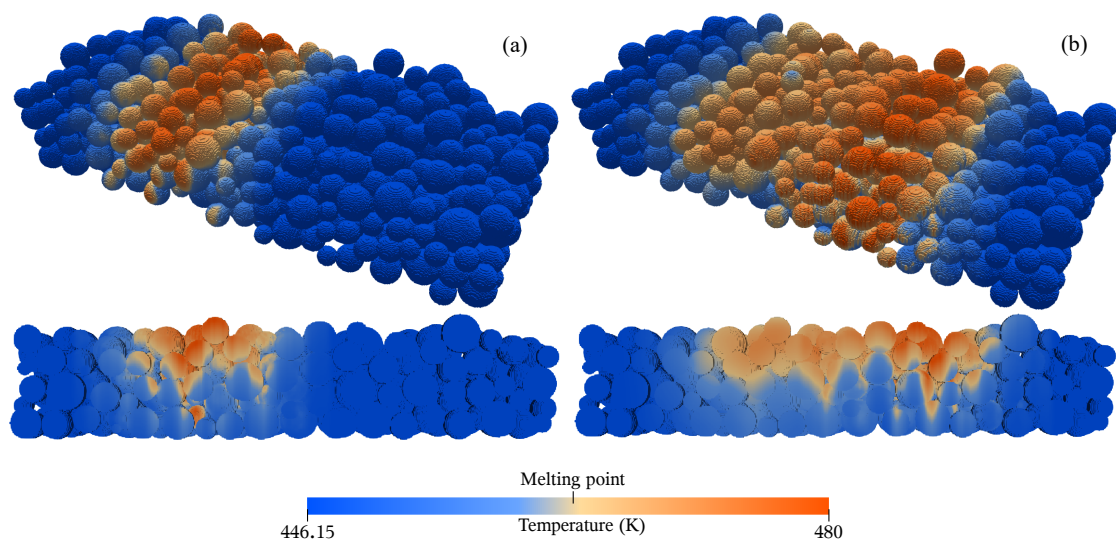


Figure 6.1: Temperature distribution after the first (a) and second (b) laser scans for the Power Decrease case.

To confirm that, the case running time was extended until no more significant increase in liquid phase fraction was observed. After just two seconds, the liquid fraction had reached its maximum, as the results in Figure 6.2 show. Figure 6.2.a, does not make a clear representation of the liquid fraction so, the same data is represented in Figure 6.2.b, but with the liquid phase as orange and the solid phase as slightly transparent blue. The results show that with the current parameters, a fusion depth of one layer (half the representative geometry height) was achieved. This information presents itself useful for cases where the only requirement for good coalescence is the particles melting. In such cases, by using these parameters instead of the lowest ones tested experimentally, a total of around 42% of energy is saved.

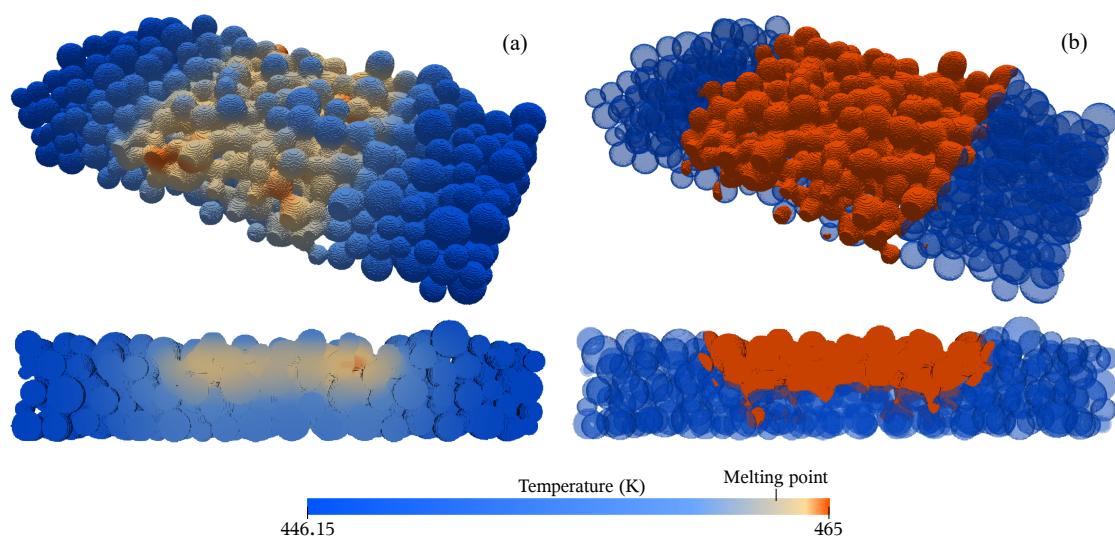


Figure 6.2: Temperature distribution after 2 seconds (a) and respective phase distribution (melted as orange and solid as blue) (b) for the Power Decrease case.

Scan Speed Increase

The scan speed that results in the same energy density of the previous case (using Equation (2.1)), but with the parameters from the base case, is 5130 mm/s. Figure 6.3 shows the temperature profile of the material after the scan. Comparing to Figure 6.1, the temperature profile is almost identical, however in this case, the maximum temperature is higher. The reason for that could be that, because the laser is moving faster and the simulation stops as soon as the scan spot fully leaves the domain, less time is given for the energy to diffuse and some cells have higher temperatures.

Theoretically, because Drexler's equation is being considered, the amount of energy received by the material is the same for both this and the previous case. Therefore, if the equation is indeed a good

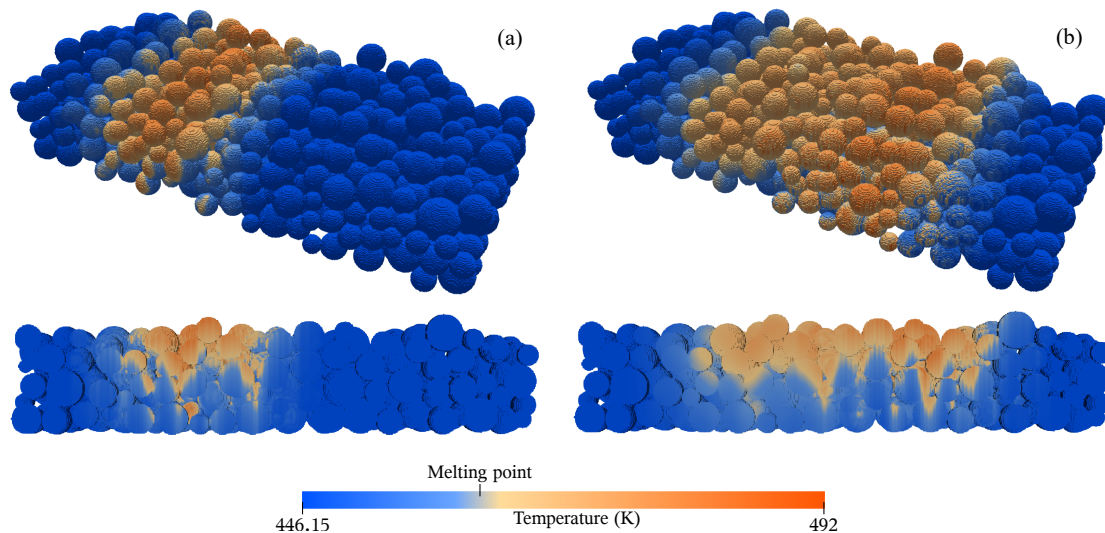


Figure 6.3: Temperature distribution after the first (a) and second (b) laser scans for the Scan Speed Increase case.

indicative of the energy received by the material, after the same time, the temperature profile and liquid fraction should be similar. Looking at Figure 6.4, it is clear that the results are not the same for identical energy density values with distinct parameters, however, they are not very dissimilar either. The case with higher speed has more energy concentrated at the core of the layer and a slightly larger molten zone. Two important conclusions can be withdrawn from these results. First, that the Drexler's equation, as mentioned previously, is a simplified approach to calculate the energy density and fails to consider some aspects. Second and last, that, although being a simplification, the results are very close, so it is not too inappropriate to use the equation, at least for cases where the parameters do not change drastically.

6.2 Hatch Distance

Adjusting the scan distance is not as straightforward as it may seem because of the laser energy Gaussian distribution. It is necessary to find the limit distance where the zones between scans will still fully melt. Being a energy density related parameter, as it was previously discussed, it is generally changed along with the scan speed and the laser power. The temperature profile of the section after the two consecutive scans is provided in Figure 6.5.

As expected, the middle point between scans received a very small amount of energy and a clear solid wall stands between the two fused zones. With the current energy parameters, it is not expected that the residual heat is enough to melt that region. Comparing with Figure 5.23, the exterior

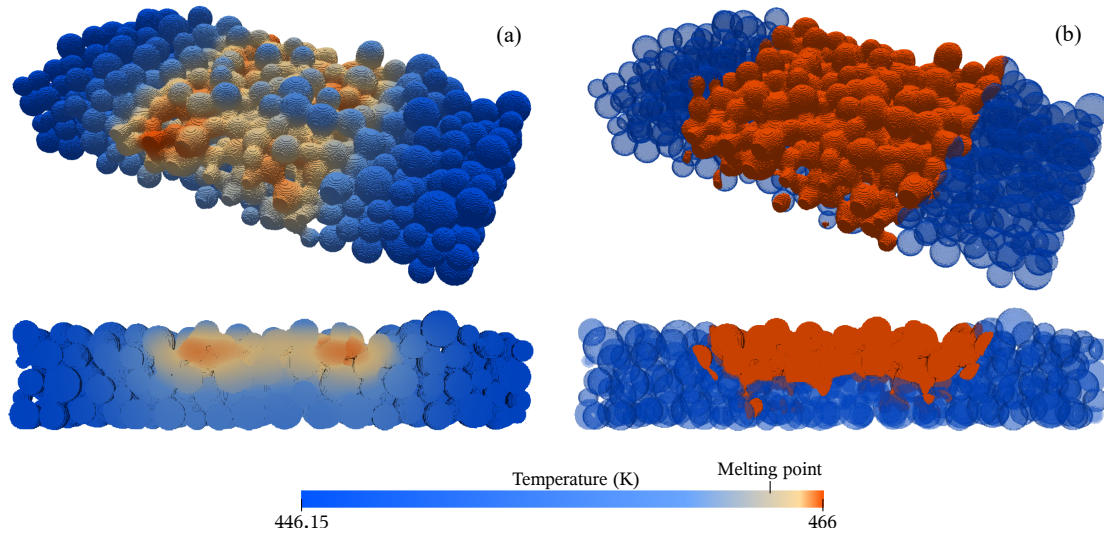


Figure 6.4: Temperature distribution after 2 seconds (a) and respective phase distribution (melted as orange and solid as blue) (b) for the Scan Speed Increase case.

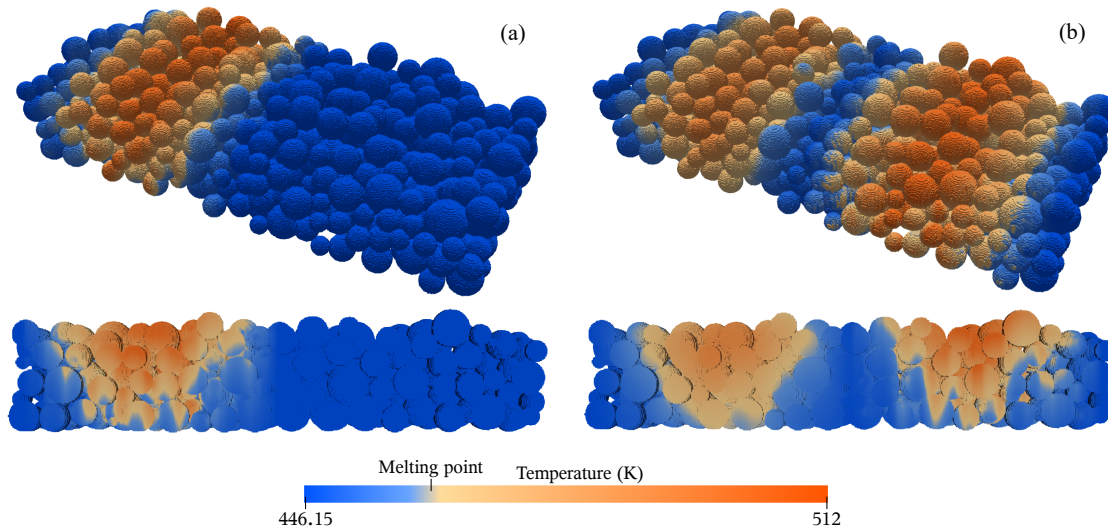


Figure 6.5: Temperature distribution after the first (a) and second (b) laser scans for the highest hatch distance increase case.

scan zones barely increase in temperature because the neighbour particles are much more cooler and quickly absorb all of the provided heat. As a confirmation, the case duration was extended and the respective results are shown in Figure 6.6. As anticipated, the residual heat was not enough to melt the particles closer to the laser scan border. The energy on the material is lost to the surrounding air and the amount that gets into the particles is not enough to surpass the phase change temperature for the entire zone. Because the temperature profile is, once again, not the most adequate form of showing the liquid fraction, since the material can be liquid below its melting point, the same data is represented in Figure 6.7, but with the liquid phase highlighted in orange. With these results, it is clear that the fused zone has reached its maximum and that, with hatch distance values of the laser diameter, there is a

significant portion of unmelted material between the scans, which obviously is not desirable.

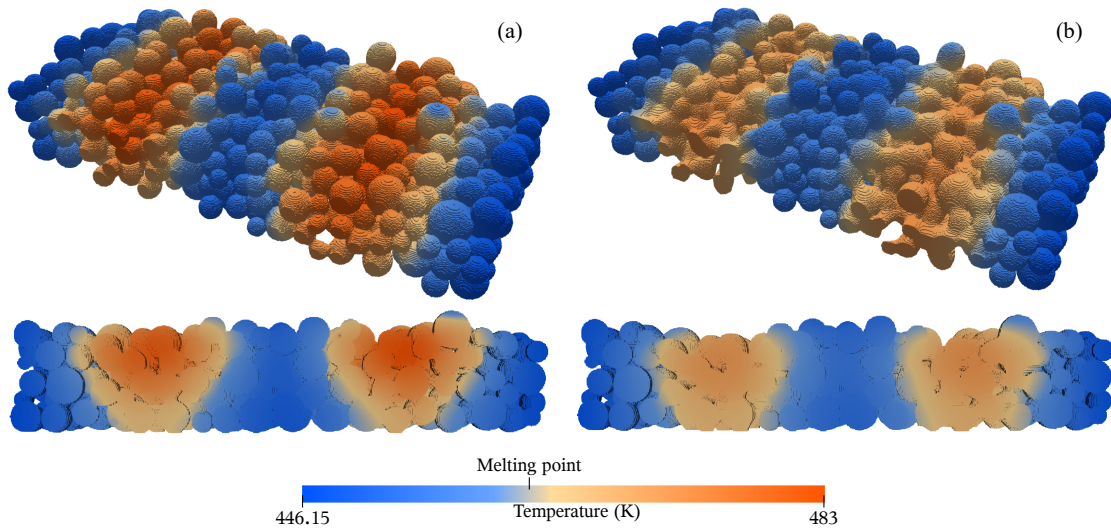


Figure 6.6: Temperature distribution after 1 (a) and 2.5 (b) seconds for the highest hatch distance increase case.

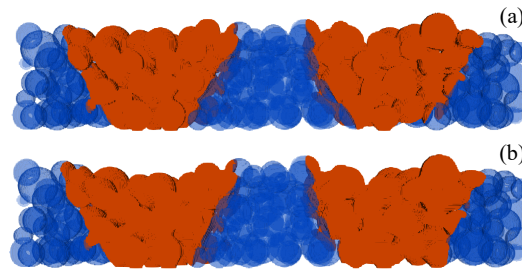


Figure 6.7: Phase distribution (melted as orange and solid as blue) after 1 (a) and 2.5 (b) seconds for the highest hatch distance increase case.

As indicated earlier, since the current scan distance was excessive, one more test is going to be performed but, this time, with a hatch distance value corresponding to half of that considered previously. The results after the first scan are displayed in Figure 6.8. By decreasing the hatch distance, there is now an overlap of molten particles right after the scan. However, this only happens at the surface, where the temperature is higher, and might not be enough to melt the remaining of the layer. Similarly to the previous analysis, the case was run for a couple more seconds until the liquid fraction increase was negligible. Looking at the temperature profile in Figure 6.9, the maximum temperature is identical to the previous case. That was expected since there is no significant overlap that would greatly increase the temperature in one zone. Moreover, despite being closer, the hot spots are very similar for both cases. The liquid fraction, displayed in orange in Figure 6.10, shows that, with this lower hatch distance, a liquid bridge, with the thickness of almost one layer, is formed between the two scanned zones. By looking at the temperature profile and comparing with the base experimental

case (Figure 5.22), the zone between scans, despite being liquid, has a lower temperature distribution, which will, most likely, cause insufficient coalescence.

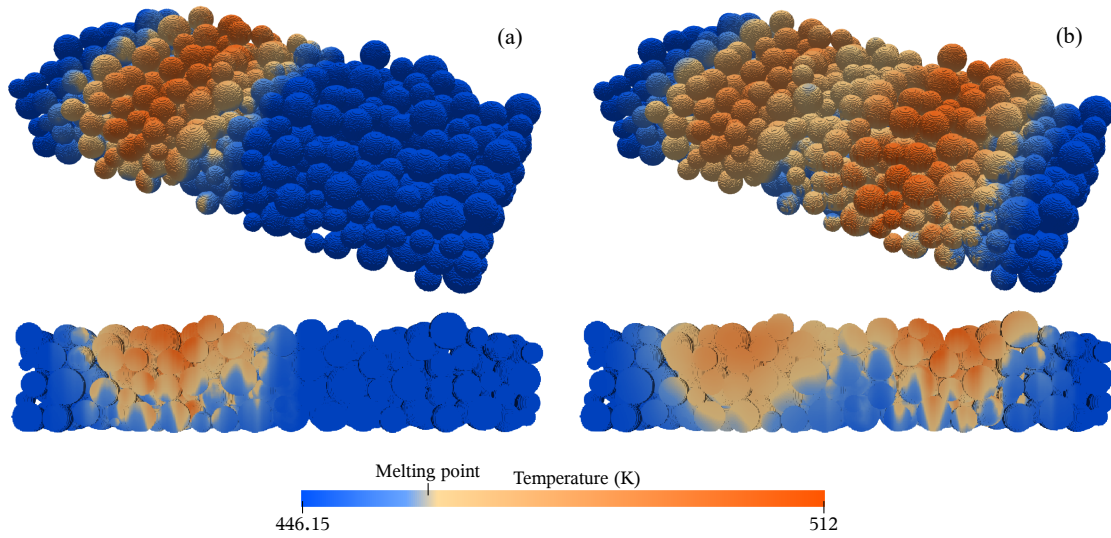


Figure 6.8: Temperature distribution after the first (a) and second (b) laser scans for the lowest hatch distance increase case.

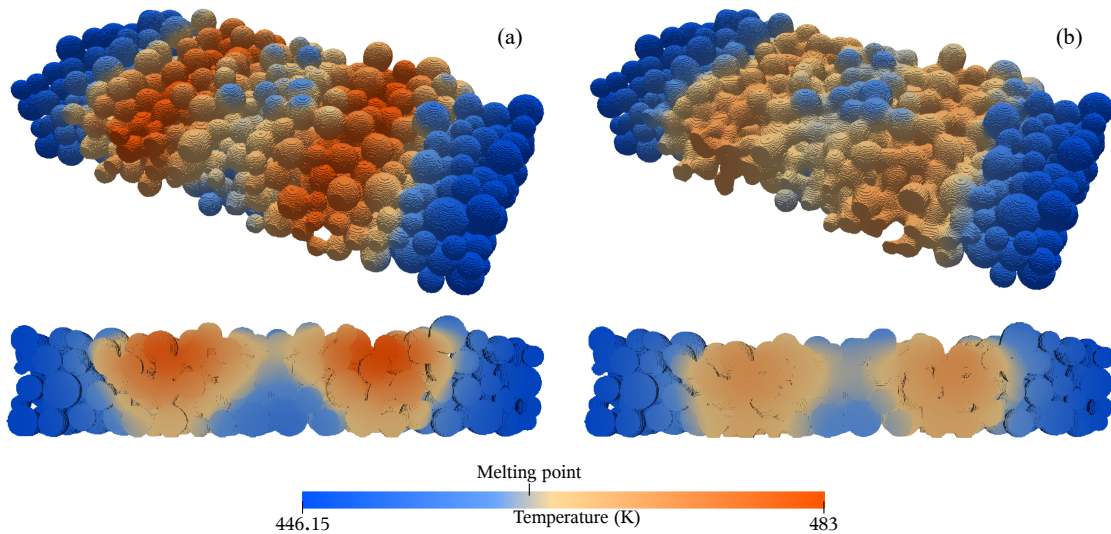


Figure 6.9: Temperature distribution after 1 (a) and 2.5 (b) seconds for the lowest hatch distance increase case.

The hatch distance increase tests prove that, for the selected energy parameters, the minimum value for a good adhesion between two consecutive scans is the starting value used in the experimental tests. This implies that, despite not being mentioned in the article of reference, some tests should have been performed to establish this parameter and 0.3 mm was found to be an appropriate, which is in agreement with the simulation results.

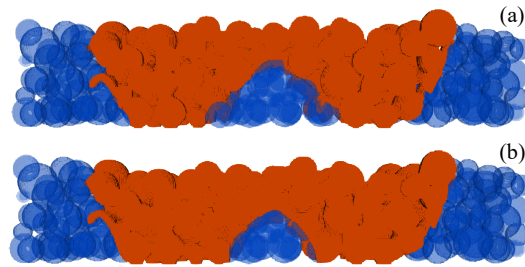


Figure 6.10: phase distribution (melted as orange and solid as blue) after 1 (a) and 2.5 (b) seconds for the lowest hatch distance increase case.

6.3 Coalescence

Two identical cases, differing only on the viscosity of the liquid phase, were extended in time in order to visualize the coalescence development.

Mixed Material

The first test (Figure 6.11) is for the mixed material viscosity (2742.5 Pa·s). This test purpose is to be a base case for comparison with the next one, where the viscosity will be increased. Unfortunately, it is not possible to evaluate the accuracy of the results in terms of coalescence since no experimental data that allowed any type of comparison was found. Nonetheless, the observed behaviour was the expected, with the coalescence increasing with time.

Used Material

The results for the increase in viscosity are illustrated in Figure 6.12. As expected, by increasing the viscosity to that of the used material, the coalesce was significantly slower. Moreover, in agreement with the tests performed in Section 5.4.1, the particles, due to the increased viscosity, retain their shape for longer and seem to be more pulled towards each other instead of mainly diffusing. Because the surface tension is modelled as a constant and the values are the same for both cases, the results are almost identical, but slower and, as seen in Section 5.4.1, eventually, the final form will be the same. This is a limitation that could be surpassed if the surface tension values for the used and virgin material were known and if the model allowed for a temperature dependent value, which would require experimental tests to determine that dependency. Assuming that these results are a correct representation, considering the simplifications employed, besides the coalesce, one can also observe

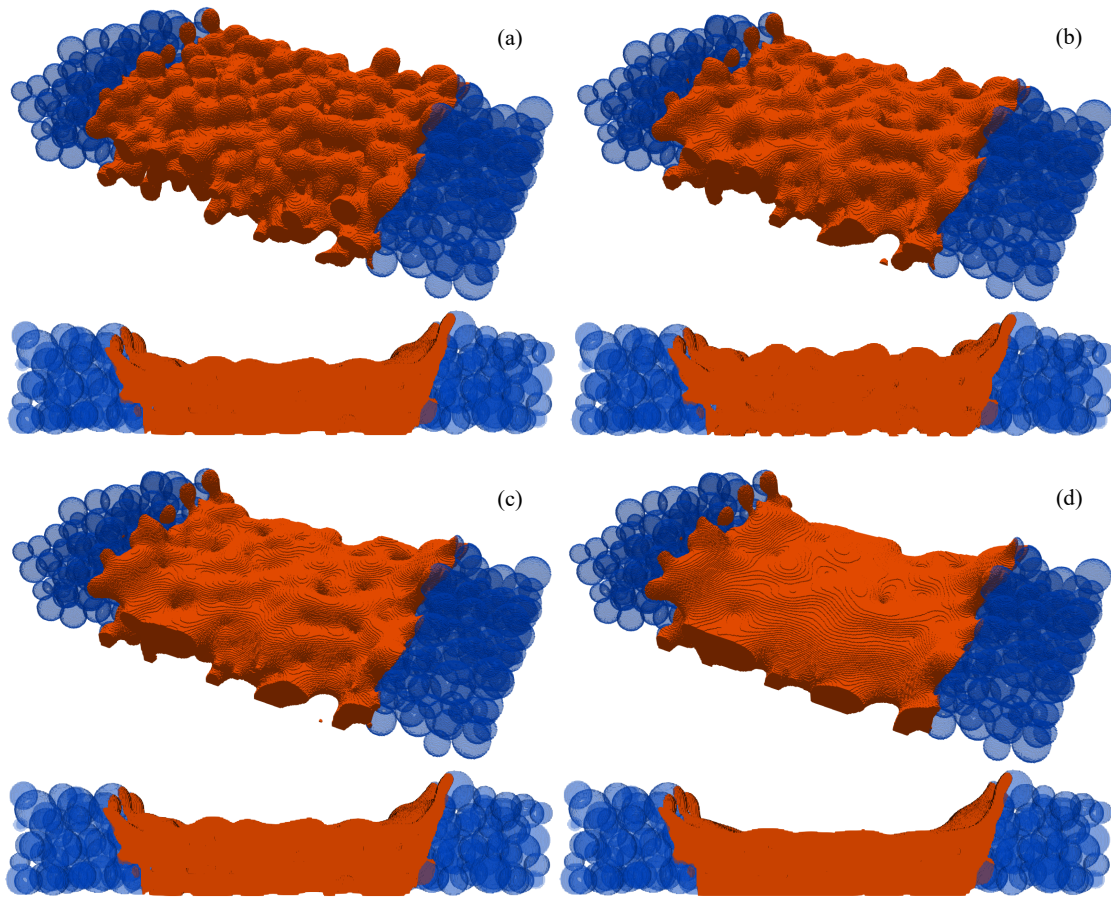


Figure 6.11: Coalescence development after 3 (a), 5 (b), 7 (c) and 10 (d) seconds for the mixed material, with the respective phase distribution (melted as orange and solid as blue).

layer densification due to the elimination of empty spaces between particles. Moreover, the partial melting of particles is also visible. The particle unmelted region will stick to the molten counterpart and that is why, in order to remove them, post processing operations, such as sand blasting [185], are often required.

6.4 Dimensional Accuracy

In preceding sections, after just a few seconds, the melted fraction reached its peak. For the other experimental cases, since the energy provided to the material was higher, a longer time for stabilization is expected. The remaining cases will also be extended past their after scan time and an analysis to the melted region will be performed to assess the part dimensional accuracy.

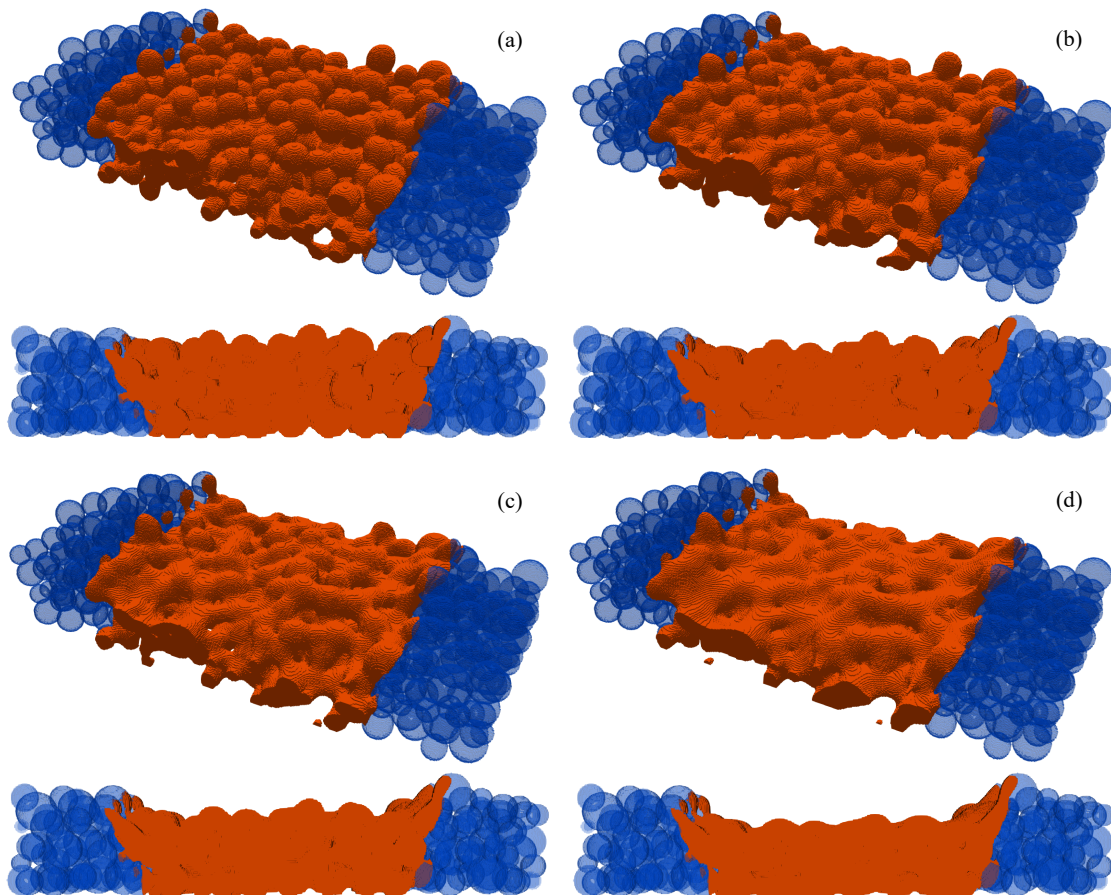


Figure 6.12: Coalescence development after 3 (a), 5 (b), 7 (c) and 10 (d) seconds for the used material, with the respective phase distribution (melted as orange and solid as blue).

Low Energy Case

The first test case, with the low energy parameters, is shown in Figure 6.13. Beyond around two thirds of the laser radius, the material remains solid. Due to the low energy density, a significant portion of the scanned zone is left unmelted, especially along the thickness.

Medium Energy Case

The medium energy case results, displayed in Figure 6.14, surprisingly, despite the great increase in laser power, do not possess a much larger liquid fraction. In fact, the maximum lateral growth is only around three quarters of the laser radius and most of the increase in fused particles is visible in the layer thickness direction. This is, most likely, motivated by the typical polymer thermal insulating behaviour.

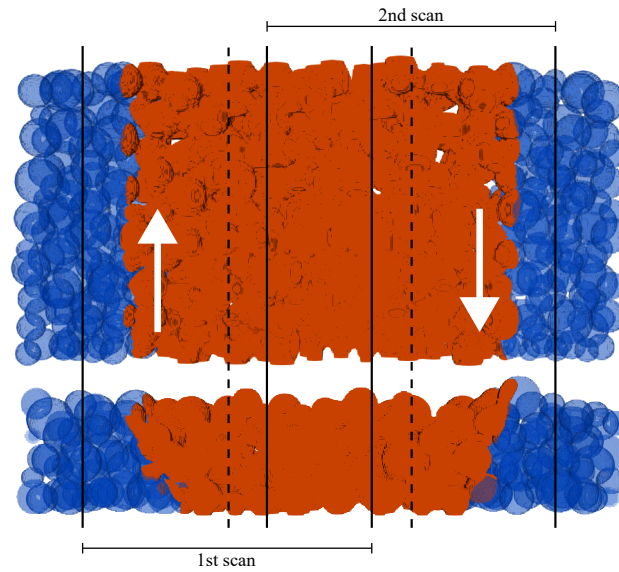


Figure 6.13: Phase distribution (melted as orange and solid as blue) in relation to the scanned zone for the low energy case.

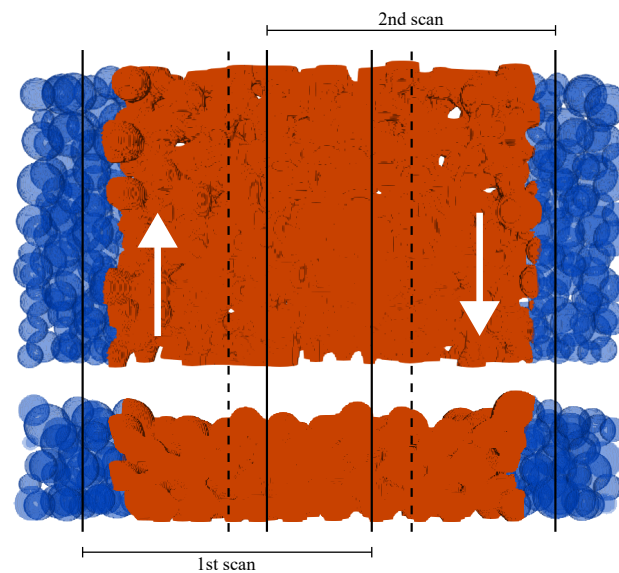


Figure 6.14: Phase distribution (melted as orange and solid as blue) in relation to the scanned zone for the medium energy case.

High Energy Case

Figure 6.15 shows the results for the high energy case. As anticipated, by increasing the laser power, more of the scanned area was able to phase change and the molten area is now closer to the scanned one. Despite the energy, for these process parameters, being so high that the material degrades, the phase fraction on the periphery of the scanned area does not increase significantly. This seems to be a consequence of the Gaussian intensity distribution that concentrates the energy at the

center of the scan in a way that, despite the laser power increase, not much of that energy reaches the periphery, and less notable changes are visible in this region, as evidenced by the temperature profiles from the tests in Section 5.6. Such behaviour indicates that the increase in width of the molten zone is mainly due to the accumulated energy at the high intensity zones that diffuses through heat conduction and not so much because the laser provides more energy at the periphery. However, the low polymer thermal conductivity, coupled with the low contact area between particles, hinders the energy diffusion. The contact area increases when the material coalesces, but that is a slow process and by the time a larger contact area is formed, most of the energy is lost through convection, as one can observe, for example, in Figure 6.9. All these reasons lead to a small lateral growth difference between the test cases, despite the distinct laser power values employed. The part growth is, most likely, a much larger concern for metal applications, since they have a much higher thermal conductivity and lower viscosity that allows for a greater contact area.

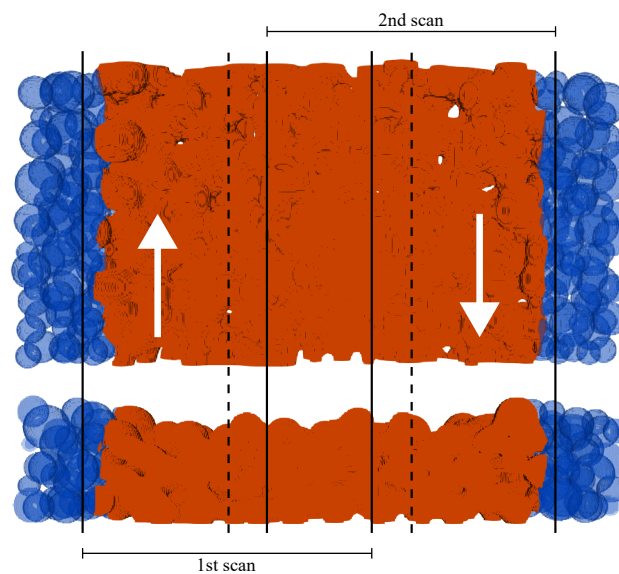


Figure 6.15: Phase distribution (melted as orange and solid as blue) in relation to the scanned zone for the high energy case.

CHAPTER 7

Conclusions and Future Work

SLS is one of the most popular AM techniques due to its capability of processing parts with complex geometries and good mechanical properties with almost no material wastage. However, the process is extremely complex due to its multi-physics nature and, as a consequence, it is yet not fully understood. There is still a significant amount of defects associated with the process and solving them experimentally has proved to be challenging, expensive and time-consuming.

Nowadays, there is commercial software that simulates the SLS process, however, they present some major drawbacks, such as the high license cost, limiting the usage to only large companies, and the low flexibility to adapt the code to the user specific needs. For those who cannot afford such costs or limitations, open-source software is viable and an interesting alternative. Unfortunately, the literature on the numerical modelling of the process is not developed enough, especially for the use of open-source software.

The present work focused on a global view of the SLS process and its simulations, with various aspects related to the process description, challenges and modelling discussed in more detail. Such analysis was necessary for the correct development of a computational tool to simulate the process at a particle length scale within an open-source framework. By using LIGGGHTS and OpenFOAM, a realistic powder bed was created and several studies were performed to assess the process evolution. Among the various studies, despite some necessary simplifications, the results were very satisfactory and in agreement with the available experimental data used for comparison. Starting with the thermal model, the laser source is behaving as expected and, based exclusively on the temperature profile after scan, the temperatures achieved by the material are a good representation of the real behaviour. The reflection model did not result in significant changes to the results, which was expected, according to the literature. Nonetheless, more efforts are needed to evaluate its adequacy and possible implementation in future simulations. Regarding the coalescence, arguably the most important phenomena on the process, several simplifications had to be employed. Starting with the viscosity of the material, it was

not possible to consider a portion of the particles with distinct viscosity levels to fully replicate the experimental practice, due to the incorrect interaction, predicted by the solver, between distinct liquid phases, thus, an average value had to be selected. Moreover, the viscosity was defined as constant, when in reality it varies significantly with temperature. By adapting the code and obtaining information on the temperature dependency of the viscosity for both the used and virgin material, a mixed powder bed could be used and the insufficient coalescence between particles, due to their high viscosity in low temperature zones, would be much more prominent and representative of the reality. Similarly, the surface tension is also treated as a constant in the current model, but if a temperature dependency was implemented, the results would likely also be more realistic. Sadly, no experimental data exists for that dependency as well.

Lastly, as a closing statement, the developed strategy, using exclusively open-source software, manifests an immense potential. The powder bed is a realistic representation of reality and the particle size distribution influence is clearly visible in the test cases. The solver is also behaving as expected and the parameters influence is evident for all the performed studies. For a future work, if efforts are put into accurately determining the material properties that could not be correctly defined and the model is adapted to accept some dependencies and behave correctly between two distinct fluids, the current methodology could become a powerful tool to further assess, with higher detail, the process parameters influence. Moreover, for further validation of the solver capability, experimental cases with specific conditions, that would allow a more rigorous comparison with the simulation results, could also be performed.

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