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Multiphysical modeling of the heating phase in the polymer powder bed fusion process



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ABSTRACT

A numerical framework based on a modified Monte Carlo ray-tracing method and the Discrete Element Method (DEM) is developed to predict the physical behavior of discrete particles during the Powder Bed Fusion (SLS) process. A comprehensive model coupling all major aspects of the underlying physics and the corresponding numerical framework, accounting for radiative heat transfer, heat conduction, sintering and granular dynamics among others, is developed. In particular, the effect of scattering on the laser-particle interaction is investigated and accounted for in the numerical framework. The spatially and temporally varying distribution of heat and displacement within the additively manufactured object are captured in detail. The model is validated through the comparison of simulated results with existing experimental results in the literature.

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1. Introduction

Additive manufacturing is an area of rapidly growing interest due to its many applications and advantages easy control and flexibility among them. Powder bed fusion (SLS), arguably the most modern and innovative non-contact additive manufacturing process, is one of the most promising techniques of additive manufacturing with a wide range of applications. Physical properties of components manufactured through the SLS process if enhanced will produce high performance parts. That can only be done if the coupled physical phenomena occurring during the SLS process are modeled with a high degree of realism, confidence and accuracy. But unfortunately several phenomena underlying the SLS process are still not well understood at this time to produce an accurate enough modeling of the process.

The goal of this paper is to develop a methodology and the corresponding numerical framework to simulate the polymer powder

bed melting process. An in-depth understanding of the multiple, coupled physical phenomena, which occur during the process, is developed and translated into a study of the relative influence of various physical factors on the properties of the final product. The simulation framework developed in this paper has the potential to lead to the manufacturing of products with higher performance through an optimization process, thus extending the areas of application of this innovative technology.

Unlike traditional technologies, the SLS process turns powders, a typical non-homogeneous granular medium into solid objects. Thermal radiation and heat conduction related to the SLS process are investigated through either continuum or discrete particle approach in the literature, Kaviani [1]. The granular bed is assumed to be a homogeneous medium with effective properties in the continuum approach even though each and every one of the physical properties of the medium is obtained separately experimentally. In contrast the discrete particle approach takes into account the discrete nature of the system, and models the packed bed explicitly.

The energy input of the laser beam into the packed bed is often simulated as a heat flux with normal (Gaussian) density distribution in the continuum approach. A three-dimensional finite element model of the process, which takes the heat flux as a boundary heat source on the surface, was developed by Lin et al. [2] to

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predict the temperature and density distributions in sintered amorphous polymer powders. Several authors based the simulation of the absorption into the material on the Beer-Lambert law, Labeas et al. [3], Grewell et al. [4] and Defauchy [5] among others. Ignoring the effect of scattering on the laser-particle interaction is not realistic given the particulate nature of the powder in the packed bed. But by and large it is not accounted for in the literature the above authors among them.

The scattering effect was accounted for in the study of the welding process of polycarbonate (PC), polyamide 6 (PA6) and glass fibers reinforced polyamide 6 (PA6GF) by laser transmission welding using an FEM based numerical simulation and experimental measurements, Mingliang et al. [6]. In their work the optical extinction coefficient is separated into two contributions: absorption and scattering. However, this approach does not take into account the redirection of photon propagation, and thus fails to paint a realistic picture of the scattering phenomenon. As early as 1988 the discontinuous approach based on the Monte Carlo and/or ray-tracing method was recommended as a natural choice for predicting radiative heat transfer in granular systems, Tien et al. [7]. A Monte Carlo method based on the Mie theory to analyze the scattering effect in a non-absorbent polymer powder bed has been used by Mariana et al. [8], followed by Zhou et al. [9] who developed a Monte Carlo method based on ray tracing to simulate the radiative heat transfer in a bimodal randomly packed structure composed of particles of various size and emissivity. The latter authors also report experimental confirmation of their Monte Carlo calculations of the light scattering in the polymeric packed bed. A numerical method based on ray tracing to simulate the light scattering during laser welding process has been proposed by Andre et al. [10]. In their work the radiative energy at the welding interface is estimated to describe the heat source. The Monte-Carlo method has been also used by Singh and Kaviany [11] to study radiative heat transfer in a mono-dispersed powder bed. They proposed a discrete ordinate method based on a scaling approach to scale independent radiative properties to obtain effective properties. A ray-tracing model is developed by Wang et al. [12] to simulate the energy absorption and penetration during the SLS of metal powders. Their model based on geometrical optics yields the evolution of the energy absorption in the powder and predicts the sintering zone dimension.

To our knowledge, most if not all studies on heat conduction in granular media in the literature are based on the FEM and on the powder bed regarded as equivalent homogeneous media, for example in Roberts et al. [13], Chen and Zhang [14] and Dai and Gu [15] among others. In these contributions the method is applied to solve the problem of heat transfer in polymeric granular media. The accuracy of this type of work relies on empirically obtained values of thermal properties of the bed. However, the variation and evolution of the powder distribution as well as the conductivity of the medium are inherent to the evolving composition and structure of the powder bed as the SLS process is unfolding and should be measured and predicted over the entire SLS process. Densification mechanism of WC/Cu powder systems during the SLS process has been studied using the finite volume method, Dai and Gu [15]. Their numerical results always overestimate experimental findings due to the embedded shortcomings of their methodology as they work with the assumption of homogeneous powder beds using empirical equations for the material characteristics. The same approach is proposed by Fischer et al. [16], in a 2D FEM model of the periodic pulses of a laser on a polymer powder. Several authors developed complex models coupling multiple phenomena based on the FEM using effective physical properties, Zhang et al. [17], Childs et al. [18], Nelson et al. [19], Bugada et al. [20], Schultz [21] among them. In summary numerical models of granular media based on the FEM are born with several limitations. They are not capable of capturing the physical behavior of grains in the powder bed,

the loss of contact between particles, or the random particle rearrangement. They also cannot capture densification caused by the escaping entrapped air between grains, and they underestimate the effect of the air between grains in the SLS process. The accuracy of these methodologies also depends on the empirical effective values of the material properties which are hard to measure and predict during the sintering process. FEM based methodologies devised to solve this problem are based on the inherent fundamental assumption of homogeneous media. However, unlike in homogeneous media heat conduction in granular media like powder beds takes place almost exclusively through physical contacts between particles, and depends strongly on the nature of the contact between individual grains. Hence, the traditional continuum model of heat conduction is not suitable in simulating the powder sintering process. Nearly all production processes of powder technology include a sintering step at a high temperature. Some of the constitutive sintering models used in the framework of continuum mechanics are derived from micromechanical models on a grain scale. In contrast the discrete elements method (DEM) represents explicitly the particulate nature of the polymer powder, and captures almost all of the physical phenomena linked to particle interactions as well as the granular characteristics of the material and thus is singularly suited to model phenomena in materials with a discontinuous structure. Heat transfer in this type of media is more realistically captured via methods based on contacts between interacting particles than those based on the assumption of homogeneous media like in the FEM based methods. However in spite of its obvious advantages the applications of the DEM in granular media in the context of the SLS process are relatively rare. One exception is the recent work of Steuben et al. [22] on the simulation of particle-based additive manufacturing demonstrating the great potential of DEM predictions in the design and characterization of additively manufactured components.

In this paper, an all-encompassing general model based on the DEM coupling all aspects of the underlying physics including radiative heat transfer, heat conduction, sintering and granular dynamics is developed. In particular a radiative heat transfer sub-model based on a modified Monte Carlo ray-tracing method accounting for the effect of scattering on the laser-particle interaction is formulated and validated by comparison with experimental results available in the literature. The model captures the behavior of discrete particles during the SLS process with great accuracy. A comprehensive example is given to demonstrate the capability of the framework developed in capturing the spatially and temporally varying distribution of heat and displacement within the additively manufactured object.

2. Global model of SLS

Unfolding physical phenomena during the SLS process are multiple and complex. A general model that takes into account most, if not all, of the physical phenomena during the SLS process is required to make reasonably good predictions of the material behavior during the process. To accomplish this goal, the model can be separated into four sub-models: the radiative heat transfer, discrete heat conduction, sintering and contact dynamics. The model structure is presented in Fig. 1.

The sub-model for radiative heat transfer in Fig. 1 uses parameters of the laser beam such as laser power, scanning speed and radius of the laser beam together with the optical properties of the material and the grain geometry to calculate the energy absorbed by the powder bed. The heat flux from sub-model of radiative heat transfer is regarded as the internal heat source in the discontinuous heat conduction sub-model. The temperature field in the powder bed is calculated via the discontinuous heat conduction sub-model,

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