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Heat and fluid flow in additive manufacturing—Part I: Modeling of powder bed fusion

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ABSTRACT

Structure and properties of components made by the powder bed fusion (PBF) additive manufacturing (AM) are often optimized by trial and error. This procedure is expensive, time consuming and does not provide any assurance of optimizing product quality. A recourse is to build, test and utilize a numerical model of the process that can estimate the most important metallurgical variables from the processing conditions and alloy properties. Here we develop and test a three-dimensional, transient, heat transfer and fluid flow model to calculate temperature and velocity fields, build shape and size, cooling rates and the solidification parameters during PBF process. This model considers temperature dependent properties of the powder bed considering powder and shielding gas properties, packing efficiency and powder size. A rapid numerical solution algorithm is developed and tested to calculate the metallurgical variables for large components fabricated with multiple layers and hatches rapidly. Part I of this article describes the model, solution methodology, powder bed properties, and model validation. The applications of the model for four commonly used alloys are presented in part II.

1. Introduction

In laser-assisted powder bed fusion (PBF) process, parts are built by progressively melting thin layers of alloy powders by a laser beam [1]. Structure and properties of these components are affected by the metallurgical variables such as transient temperature fields, cooling rates and solidification parameters. These metallurgical variables depend on process parameters such as laser power, wavelength, power distribution, travel speed, layer thickness, hatch spacing, powder shape and size and the alloy used [1]. Currently, the structure and properties of the components are often optimized by trial and error without any guiding scientific framework. This method is expensive, time consuming, and provides no assurance of achieving the desired product attributes [2,3]. A recourse is to develop, test and utilize theoretical models that enable users to specify various additive manufacturing (AM) process parameters and alloy properties to obtain the important metallurgical variables such as the transient temperature fields, cooling rates and solidification parameters. In short, when adequately tested with experimental data, these models help to fabricate defect free, structurally sound and reliable components based on scientific principles.

Several attempts have been made to calculate important metallurgical variables in PBF. Finite element based heat conduction models [4,5] can calculate temperature fields, build shape and size, cooling rates and solidification parameters. However, these models neglect the effects of the convective flow of liquid metal inside the molten pool driven by the surface tension gradient on the top surface of the pool. Since convection is the main mechanism of heat transfer within the liquid pool, such calculations result in erroneous temperature gradients, unrealistic cooling rates and solidification growth rates. Manvatkar et al. [6] showed that the cooling rates are overestimated by a factor of two when the molten metal convection is ignored during laser-assisted direct energy deposition. Heat transfer and fluid flow models [7,8] are computationally intensive and various simplifications are often made to make them tractable. Careful consideration of thermophysical properties of the powder bed taking into account powder size and/or packing efficiency is needed to correctly simulate experimental results. Powder scale models [9–12] using level set method or volume of fluid method consider both molten metal convection and correct powder bed properties. However, these models are computationally intensive and often restricted to two-dimensional calculations. In addition, they have not been applied to examine the manufacture of real components with multiple layers and hatches.

Here, we develop and test a three-dimensional, transient heat transfer and fluid flow model for multiple layers and hatches PBF process. The model solves the equations of conservation of mass, momentum and energy in transient, three-dimensional form. These governing equations are

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discretized using control volume method in a solution domain that consists of the substrate, powder bed and solidified build. Effects of the molten metal convection are considered in the calculations. The temperature dependent thermo-physical properties of the powder bed are calculated considering the size of the powder and packing efficiency of the powder bed. A traveling grid system along the direction of scanning has been developed to achieve high computational efficiency while limiting memory requirements for the simulation of large transient problems in builds involving multiple layers and hatches. The calculated results are compared with independent experimental data.

Due to the complexity of the problem and the applicability of the traveling grid algorithm to save computational time and memory requirements in large related three-dimensional transient problems, the work is divided into two parts. In this paper (part I) the development of the model, discretization of the governing equations, calculation of powder bed properties and the development and testing of a computationally efficient solution technique are presented. In an accompanying paper (part II) the application of the model to laser-assisted PBF of four commonly used alloys, stainless steel 316, Ti-6Al-4V, Inconel 718 and AlSi10Mg are discussed.

2. Numerical heat transfer and fluid flow model

The solution domain consists of the substrate, powder bed and multi-layer multi-hatch build as shown in Fig. 1. The scanning, hatching and building directions are indicated by X, Y and Z, respectively. For simplicity, unidirectional scanning strategy is used where the laser beam travels only along the positive X-direction for all layers and hatches. After a particular hatch is completed, the laser beam shifts along the positive Y-axis by a distance equal to the hatch spacing. After the completion of all hatches in a particular layer, the laser beam shifts along the positive Z-axis by a distance equal to the layer thickness since the powder bed is lowered by the same distance in the actual process. The same process continues until all hatches and layers are completed. Heat transfer calculations are done in the entire solution domain. However, fluid flow calculations are restricted inside a smaller domain containing the molten pool and its adjacent regions to save the total computational time.

2.1. Assumptions

The following simplifying assumptions are made to make the computational work tractable.

(a) Densities of powder, solid and liquid alloys are assumed to be independent of temperature except for the calculation of the buoyance force. This assumption is known as the Boussinesq approximation and is widely used in the calculations of buoyancy driven flow [2,13].
(b) The surfaces of the growing layers and hatches are assumed to be flat.
(c) The liquid metal flow is assumed to be incompressible and Newtonian. The turbulent flow in the molten pool is considered through the use of the enhanced thermal conductivity and viscosity of the liquid metal [14].
(d) The loss of alloying elements due to vaporization [15] and its effects on both heat loss and composition change are not considered in the calculations.

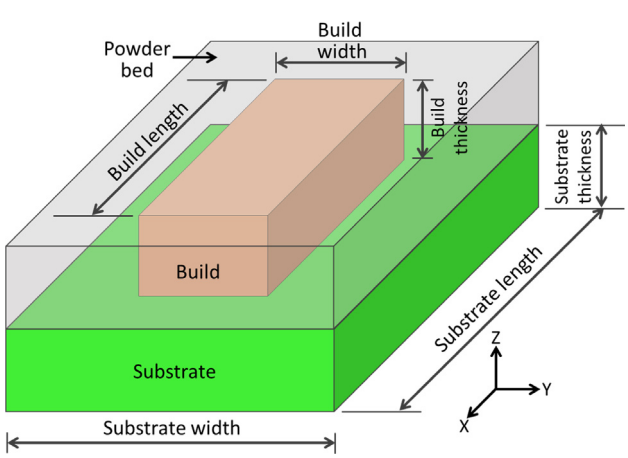

Fig. 1. Schematic of the solution domain consisting of substrate, powder bed and build. X, Y and Z directions represent the scanning, hatching and building directions, respectively.

2.2. Governing equations and volumetric heat source

The heat transfer and fluid flow model is applied in a 3D Cartesian co-ordinate system and it solves the equations of conservation of mass, momentum and energy [15–18] to calculate enthalpy, three components of velocity and pressure.

By dividing the total enthalpy into the sensible heat and the latent heat of fusion, the energy conservation equation is written as:

$$\frac{\partial h}{\partial t} + \frac{\partial (u_i\ h)}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\alpha \frac{\partial h}{\partial x_i}\right) - \frac{\partial \Delta H}{\partial t} - \frac{\partial (u_i\ \Delta H)}{\partial x_i} + S_v \tag{1}$$

where h is the sensible heat, t is the time, α and ΔH are the thermal diffusivity and the latent heat of fusion of the alloy, respectively, u_i and x_i are the velocity components and the distance along the i direction, respectively and S_v is the source term to account for the volumetric heat source. In PBF-AM, the laser beam undergoes multiple reflections inside the powder layers [1]. Therefore, a 3D volumetric heat source is considered here. The heat source is characterized by the laser power (P_L), laser beam radius (r_b) and a power distribution factor (d):

$$S_v = \frac{d\ \epsilon\ P_L}{\pi\ r_b^2\ \lambda} \exp\left[-\frac{d\ (x_b^2 + y_b^2)}{r_b^2}\right] \tag{2}$$

where x_b and y_b are the X and Y distances from the axis of the laser beam, respectively and λ is the powder layer thickness. The distribution factor, d varies between 1 and 3 depending on the spatial distribution of the power of the laser beam on a particular XY-plane [1]. The higher the distribution factor, the higher the peak power. The distribution of the laser power is uniform along z-direction throughout the powder layer thickness and ϵ is the heat absorption coefficient. The absorption co-efficient is high inside the powder layer due to the multiple reflections of the laser beam. For example, a value of $\epsilon = 0.7$ was reported for stainless steel 316 [1]. However, as the powder melts the absorption coefficient drops to the Fresnel absorptivity, which is 0.3 for stainless steel 316 irradiated by a Nd-YAG laser [1].

Velocities of the metal inside the molten pool are calculated by solving the following momentum conservation equation.

$$\rho \frac{\partial u_j}{\partial t} + \rho \frac{\partial (u_i\ u_j)}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\mu \frac{\partial u_j}{\partial x_i}\right) + S_j \tag{3}$$

where ρ and μ are the density and the viscosity of the alloy, respectively, u_i and u_j are the velocity components along the i and j directions, respectively and S_j is the source term for jth momentum conservation equation. Spatial gradient of the pressure field is responsible for the generation of the convective flow of liquid metal inside the molten pool. The following continuity equation is solved in conjunction with the momentum conservation equation to obtain the pressure field.

$$\frac{\partial u_i}{\partial x_i} = 0 \tag{4}$$

The driving forces of the molten metal convection include the surface tension gradient on the top surface of the pool and the buoyancy

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