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3-Dimensional heat transfer modeling for laser powder-bed fusion additive manufacturing with volumetric heat sources based on varied thermal conductivity and absorptivity

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HIGHLIGHTS

- Eight 3D heat sources used for simulating Laser Powder-Bed Fusion are compared.
- New equations for varied thermal conductivity and laser absorptivity is proposed.
- The varied thermal conductivity and absorptivity expressions can be linear functions.

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ABSTRACT

In this article, a 3-dimensional heat-transfer finite element model for Laser Powder-Bed Fusion (LPBF) was developed for accurately predicting melt pool dimensions and surface features. The sole deployment of trial-and-error experiments for arriving at optimal process parameters is very costly and time-consuming, thus the developed model can be used to reduce the process/material development costs. A literature review of heat source models was presented. Eight commonly used heat source models are evaluated and compared. All of their simulated depths are smaller than the experimental result, which may be due to the melt pool convection and inconstant laser absorptivity in the reality during the experiment. In order to enable the numerical model to predict melt pool dimensions for different combinations of process parameters, a novel model including expressions of varied anisotropically enhanced thermal conductivity and varied laser absorptivity is proposed and verified by both the melt pool dimensions and track surface morphology. It is found that the heat source expressions can be linear while causing the simulation results to be in better agreement with both experimental melt pool dimensions and track surface morphology.

1. Introduction

Laser Powder-Bed Fusion (LPBF) is a commercially available Additive Manufacturing (AM) process. It is regarded as one of the most common processes for direct metal fabrication [1]. In LPBF, geometrically complex parts can be produced by selectively melting layers of powder. Nevertheless, wide industrial applications of LPBF are hindered by several limitations, including porosity defects resulted from lack of fusion, keyhole collapse, and balling [2], and residual stress which causes distortion and failure of the final products due to high thermal gradients [3,4]. Therefore, machine process parameter optimization becomes a critical task.

However, the sole deployment of trial-and-error experiments to

determine optimal process parameters is very costly and time-consuming [5] since there will be a large number of coupon samples with different combinations of process parameters, such as laser power, scanning speed, powder layer thickness, hatch spacing, preheating temperature, and scanning patterns. Therefore, numerical simulations of the LPBF process are widely investigated.

The physical phenomena associated in a melt pool are highly complicated, mainly controlled by mass and heat transfer. The heating and cooling rates are extremely high due to the fast-moving laser irradiation on the powder particles [6]. In addition, the dynamic melt pool development beneath the powder-bed [7], phase change dynamics from liquid to vapor and plasma [8], and powder particles drawn by high-speed metal vapor flux [9] and capillary effects exist in the melt

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pool. Therefore, fine-scale numerical models [10,11], which included several details, such as laser-ray tracing in randomly distributed particles and thermal fluid dynamics, have been built in order to simulate several complex melt pool behaviors. However, the computational cost for such simulations is extremely high. For example, the work done in [10] employed ALE3D (developed in Lawrence Liverpool National Laboratory) massively-parallel code which consumes on the order 100,000 CPU-h [5], and the work done in [11] took 140 h for only 4 ms simulation of the process.

Therefore, for reducing the computational time, effective simulation models with certain approximations and assumptions to predict the dimensions of melt pools (e.g. melt pool width and depth) have been proposed. For simplification, instead of employing laser-ray tracing method in randomly distributed particles, the heat source has been usually assumed as volumetric heat source models, and the powder layer is presumed as homogeneous bulk materials with effective powder-layer material properties. In the literature, researchers have employed various heat sources. These heat sources can be categorized into two groups based on their characteristics, namely (a) Geometrically Modified Group (GMG); and, (b) Absorptivity Profile Group (APG). In GMG, different geometries are used to mimic the actual shape of the heat source, such as cylinder shape [12], semi-sphere [13], semi-ellipsoid [13,14], and conical shape [15]. For example, the work in [12] built up a volumetric heat source model with the consideration of the optical-penetration depth (OPD) of the laser beam into the powder-bed, where the shape of the heat source is a cylinder. Bruna-Rosso et al. [14] implemented the semi-ellipsoid heat source model, which was proposed firstly by Goldak et al. [13], in the LPBF simulation. The model showed good agreement with the experimental results. Wu et al. [15] proposed a conical shape of the heat source for arc welding, which is comparable to the LPBF process, and derived a good set of data in accordance with experimental results. On the other hand, in APG, the powder-bed of LPBF is viewed as an optical medium and the laser beam is assumed to be absorbed gradually along the depth of the powder layer. Therefore, several absorptivity profiles have been proposed, such as radiation transfer equation [6], absorptivity derived by the Monte Carlo method [16], linearly decaying equation [17], and exponentially decaying equation [18]. In APG, the heat source models are not constrained in specific geometries, and their general form is that two-dimensional Gaussian distribution is on the top surface while the laser beam is absorbed along the depth of the powder-bed based on the absorptivity functions. Gusarov et al. [6] presented a mathematical approach for effectively estimating the laser radiation scattering and absorption in powder layers and developed a volumetric heat source based on the radiation transfer. In the work done in [18], a heat source model was presented, which follows a Gaussian profile on the Cartesian coordinates, and an exponentially decaying profile along the z-direction. The effective heat source models presented in the literature are computationally efficient and accurate while being compared to the corresponding experimental results. However, a comparison report is not found in the literature. Heat source modeling is regarded as one of the key factors that influence not only the melt pool dimensions but also thermal variables [18], e.g. the cooling rate, etc. Therefore, comparisons of heat sources used in simulation of the LPBF process are necessary.

In addition to computation acceleration, thermal fluid dynamics, such as mass convection in the melt pool during LPBF, can be approximated effectively by the anisotropically enhanced thermal conductivity method [19]. The anisotropically enhanced thermal conductivity method could effectively improve the prediction precision of melt pool dimensions. However, its further investigation is still critical since it may be changed from one set of process parameters to others. Lastly, laser absorptivity is one of the most uncertain parameters during the numerical modeling as discussed in [5,6]. All the simulation models mentioned in the above literature employed constant absorptivity, which may not be the case in reality. The laser absorption factor is

influenced not only by the powder particle size and distribution but also the angle of incidence that varies due to the dynamic melt pool surface [20]. Trapp et al. [20] and Matthews et al. [21] studied the absorptivity in LPBF using experimental approaches. The variation of absorptivity was observed very large from 0.3 up to near 0.7 dependent on process parameters. As seen in their results, for specific range of process parameters, the absorptivity was directly proportional to the laser power. However, there is still a lack of clear expressions correlating the absorptivity and the process parameters. Besides, investigations on more different kinds of materials are still needed.

Therefore, the present study gives a summary and comparison of the heat source models commonly used by researchers in the literature. In addition, to the authors' best knowledge, it is the first attempt to develop a model including expressions of varied anisotropically enhanced thermal conductivity and varied laser absorptivity. For the model validation, melt pool dimensions and track surface morphology, e.g. track stability [22] and ripple angle [18] can be used as significant indicators since they determine the final product quality and can be quantified by experimental results at the same time. Thus, the validity of the proposed approach is verified by the melt pool dimensions and track surface morphology.

2. Background to heat transfer modeling utilized in LPBF

2.1. Governing equations

The governing expression for 3D heat transfer processes can generally be as follows,

$$\rho c \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left(k_x \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(k_y \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left(k_z \frac{\partial T}{\partial z} \right) + Q(x, y, z, t) \quad (1)$$

where ρ is the material density [kg/m³], c is the specific heat [J/kgK], T is the current temperature [K], t is the time [s], x , y , and z are the coordinates in the reference system [m], k_x , k_y , and k_z are the thermal conductivity [W/mK] of x , y , and z -axis direction, and $Q(x,y,z,t)$ is the internal heat generation per unit volume [W/m³].

Because of the preheating of the substrate, the initial temperature (T_{base}) of the substrate and the powder layer was considered as 353 [K]. The ambient temperature (T_0) distribution of the environment during LPBF can be set to 293 [K].

Convective heat losses (q_c) were considered as follows,

$$q_c = -h_c(T_{\text{sur}} - T_0) \quad (2)$$

where h_c is the convective heat transfer coefficient [W/(m² K)], and T_{sur} is the surface temperature [K].

Radiative heat losses (q_r) were accounted for by using Stefan-Boltzmann law:

$$q_r = -\varepsilon\sigma(T_{\text{sur}}^4 - T_0^4) \quad (3)$$

where ε is the emissivity of the powder-bed, and σ is Stefan-Boltzmann constant for radiation.

2.2. Heat source models

It is important to establish an appropriate heat source model of LPBF simulations since the heat source will not only influence the geometries of melt pools but also probably have an impact on the mechanical performance of final products. Heat source models used in LPBF simulations is a laser beam which is usually assumed to be two-dimensional Gaussian [23]. The beam irradiance at any point (x, y) at time t for the fundamental transverse electromagnetic mode (TEM₀₀) can be expressed as,

$$I(x, y, t) = \frac{2\beta P}{\pi r_l^2} \exp \left[-2 \frac{(x-v \cdot t)^2 + y^2}{r_l^2} \right] \quad (4)$$

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