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Mesoscopic Computational Fluid Dynamics Modelling for the Laser-Melting Deposition of AISI 304 Stainless Steel Single Tracks with Experimental Correlation: A Novel Study

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Citation: Ur Rehman, A.; Mahmood, M.A.; Pitir, F.; Salamci, M.U.; Popescu, A.C.; Mihailescu, I.N. Mesoscopic Computational Fluid Dynamics Modelling for the Laser-Melting Deposition of AISI 304 Stainless Steel Single Tracks with Experimental Correlation: A Novel Study. *Metals* **2021**, *11*, 1569. <https://doi.org/10.3390/met11101569>

Academic Editor:
Christian Mittelstedt

Received: 6 September 2021

Accepted: 27 September 2021

Published: 30 September 2021

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Abstract: For laser-melting deposition (LMD), a computational fluid dynamics (CFD) model was developed using the volume of fluid and discrete element modeling techniques. A method was developed to track the flow behavior, flow pattern, and driving forces of liquid flow. The developed model was compared with experimental results in the case of AISI 304 stainless steel single-track depositions on AISI 304 stainless steel substrate. A close correlation was found between experiments and modeling, with a deviation of 1–3%. It was found that the LMD involves the simultaneous addition of powder particles that absorb a significant amount of laser energy to transform their phase from solid to liquid, resulting in conduction-mode melt flow. The bubbles within the melt pool float at a specific velocity and escape from the melt pool throughout the deposition process. The pores are generated if the solid front hits the bubble before escaping the melt pool. Based on the simulations, it was discovered that the deposited layer's counters took the longest time to solidify compared to the overall deposition. The bubbles strived to leave through the contours in an excess quantity, but became stuck during solidification, resulting in a large degree of porosity near the contours. The stream traces showed that the melt flow adopted a clockwise vortex in front of the laser beam and an anti-clockwise vortex behind the laser beam. The difference in the surface tension between the two ends of the melt pool induces “thermocapillary or Benard–Marangoni convection” force, which is insignificant compared to the selective laser melting process. After layer deposition, the melt region, mushy zone, and solidified region were identified. When the laser beam irradiates the substrate and powder particles are added simultaneously, the melt adopts a backwards flow due to the recoil pressure and thermocapillary or Benard–Marangoni convection effect, resulting in a negative mass flow rate. This study provides an in-depth understanding of melt pool dynamics and flow pattern in the case of LMD additive manufacturing technique.

Keywords: 3D printing; laser-melting deposition; melt flow; thermocapillary or Benard–Marangoni convection force; recoil pressure; flow pattern; mass flow rate directions

1. Introduction

Figure 1 shows a schematic for laser–powder stream–substrate interaction. With the simultaneous addition of powder particles, a significant portion of the laser beam is absorbed. In contrast, the substrate absorbs a part of the laser beam to generate a melt

pool [1]. The powder particles experience in-flight and melt-pool heating, which causes phase transformation, resulting in layer deposition [2].

Figure 1. LMD schematic.

This method is often referred to as direct energy deposition (DED), laser-engineered net shaping (LENS), laser-melting deposition (LMD), laser-additive manufacturing (LAM), or direct metal deposition (DMD). Since the 1970s, this method has been used in the industrial sector, and the significance of the Marangoni effect is universally acknowledged. It is indeed clear that the melt pool evolution is still not completely understood, as it has not been investigated precisely. The Marangoni effect explains how melt on the interface flows from low-surface-tension areas to high-surface-tension regions. Since surface tension is dependent on temperature, and changes with the elemental formulation of its materials, it may be produced by an asymmetrical temperature profile, or even by a concentration gradient [3]. Because surface tension reduces with increasing temperatures, melt pool movement is driven from the middle of melt pool, with the greatest temperature, to the cooler melt pool borders.

Several experiments have been carried out to characterize the melt flow in various laser–material interaction processes. In the case of laser melting, Zhao et al. [4] illustrated that the whole flow pattern could even be inverted, owing to increased oxidation—mainly at the melt pool surfaces—which changes the surface tension’s temperature coefficient. Moreover, the buoyancy force acts upon that melt pool due to the heterogeneous temperature field, which causes varying densities within the melt pool. Tanaka [5] discovered that during the laser melting, the melt pool speed ascribed exclusively to the buoyancy effect is 10 times less than the speed produced by the surface dynamics of Marangoni shear stresses and arc-induced drag. Kumar and Roy [6] explored the laser cladding process, and found that the impact of buoyancy forces could be neglected. Furthermore, Han et al. [7] illustrated that powder infusion does have at least a localized effect on the melt pool due to particle momentum upon landing, as shown by modeling of powder particle collision. However, according to Gasser [8], the impact of shield or carrier gases on the resultant shear stress within the melt pool layer, as well as its cooling influence, can be ignored. It was further found that the melt pool’s convective current is essential in order to achieve uniformity in laser alloying applications. However, Mazumder [9] found that the convective current is responsible for the formation of pores. It is worth mentioning that

experimental techniques are expensive, and cannot provide in-depth information regarding melt flow during the deposition process. To solve this issue, one of the most commonly used techniques is the development of a simulation model.

Various simulation models have been taken into consideration to simulate the melt flow. Hoadley and Rappaz [10] developed a finite element (FE) model for the laser cladding process relying on two-dimensional (2D) heat conduction and momentum balance equations. The model was able to simulate the molten metallic clad deposition. Picasso and Rappaz [11] proposed two methods to model the laser cladding processes in 2D and 3D. The model was able to calculate the geometry of the melt pool precisely. Toyserkani et al. [12] constructed a 3D transient FE model of laser cladding with simultaneous injection of powder particles; the developed model estimated the correlations between laser scanning speed, powder particle feeding rate, and deposited layer dimensions. The impact of the moving laser beam resulted in fluid convection, which was included by changing the thermal conductivity of the layer. Choi et al. [13] developed a numerical model encompassing the majority of the cladding phenomena. A volume of fluid (VOF) modelling technique was used to forecast the melt pool flow field development. For simplicity of simulation, the feeding of metal droplets was applied instead of powder particles. Furthermore, the constant material characteristics were utilized for both liquid and solid metal. Wen and Shin [14] proposed a novel 3D model describing the coaxial laser deposition that takes into account physical phenomena including laser–powder interactions, flow pattern, mass transfer, and solidification; one of the biggest flaws of this model is that it does not take into consideration the impact of surface-active components on melt pool convection and morphology. Marangoni convection patterns produced by surface-active components are recognized to have significant impacts on melt pool morphology. For this purpose, various studies have been conducted to investigate these implications. The influence of heat and material on the surface tension of the Ni–S system was investigated by Sahoo et al. [15] and Lee et al. [16], who presented temperature-dependent surface tension and gradients using electron beam melting in the case of two different IN718 formulations (20 ppm S, 8 ppm O; and 6 ppm S, 10 ppm O). Su and Mills [17] generated an analytical surface tension model for IN718 by varying sulfur and oxygen contents at the ppm scale. Zhao et al. [18] investigated the effects of oxygen and heating on the surface tension of stainless steel.

In previous studies on laser cladding models, wherein mass additions to the melt pool are addressed, the impact of surface-active components and related convection trends on the melt pool was not considered. Until recently, the underlying behaviors of melt pools during the laser cladding process have not been thoroughly studied, i.e., the surface melt pool movement has not been examined using computational data analysis. The purpose of this article is to explain the development of a dynamic 3D mathematical model of the laser cladding method, the comparison of the model with experimental measurements, and to investigate the forecasted melt pool convective flow patterns. The following sections analyze the underlying complex principles and numerical simulations used to depict the laser cladding process, the VOF mathematical simulation approach, modeling observations of a full rotation, single-layer clad deposit geometry, and analogies to experimental data. For this paper, a method to track the flow behavior across the entire melt pool was devised in the LMD process. The flow behavior of the whole melt pool was uncovered. The driving factors of liquid flow and the fundamental processes were investigated throughout the melt pool. Moreover, the corresponding flow driven by the Marangoni effect is explained through the mass flow rate.

2. Materials and Methods

2.1. Computational Fluid Dynamics (CFD) Modelling

The powder development and deposition process computation can be separated into two steps: (a) initially, a range of particles falls simultaneously along with the laser beam, and (b) the powder particles experience in-flight and within-the-melt-pool heating. For powder particles, an interaction method with the non-linear Hertz–Mindlin elastic equation

is used to measure the elastic actual contact force [19]. At the same time, the damping factor is applied to acknowledge the dissipation of mechanical energy [20–22]. Natural contact force and damping force coexist in elastic materials: and overlap between such interacting particles takes place in the perpendicular plane. The relative stiffness throughout the plane is perpendicular. Furthermore, Young's modulus and the mass are equal. No micro-slip approach is introduced in the tangential route to accommodate the elastic contact force [19]. For this study, the flow science discrete element modelling (FS-DEM) module FLOW-3D, Santa Fe, New Mexico, USA [23], was used to model the deposition process of AISI 304 stainless steel powder particles on AISI 304 stainless steel substrate. The powder layer was deposited using discrete microparticles. Figure 2a,b show a comparison of powder particle distributions attained via scanning electron microscopy (SEM), ApreoS instrument (Thermo Fisher Scientific, Waltham, MA, USA), and the aforementioned software, respectively. The powder particles were within in the range of 45–130 μm , as can be seen in Figure 2a, while the simulated powder distribution achieved through the model is exhibited in Figure 2b. Furthermore, the particle size distribution histogram is presented in Figure 2c. For simulations, a range of the powder particles' size distribution was taken into consideration.

Figure 2. AISI 304 stainless steel powder distribution: (a) scanning electron microscopy at $150\times$ magnification, (b) simulation with a range of 45–130 μm , and (c) particle size distribution histogram of the simulation.

The LMD process involves the rapid melting and solidification of a given material, which affects all of its thermophysical properties. For the CFD model, temperature-dependent thermophysical properties of AISI 304 stainless steel with phase changes were measured using FLOW-3D CFD software, based on the chemical composition provided in Table 1.

Table 1. Chemical composition of AISI 304 stainless steel powder particles [24–26].

Element	C	Cr	Mn	Si	P	S	Ni	N	Fe
Composition	0.07%	17.5–19.5%	2.0%	1.0%	0.045%	0.015%	8.0–10.5%	0.10%	Balance

A CFD framework was developed and implemented using particular subprocesses of the FLOW-3D CFD program. For simplicity, the research estimates several variables and generalizations: (a) the melting across the melt stream is assumed to be incompressible Newtonian, and (b) the change in mass owing to metal evaporation is often ignored. Equations (1)–(3) are solved for mass continuity, momentum, and energy conservation, respectively:

$$\nabla \cdot \vec{v} = 0. \quad (1)$$

$$\frac{\partial \vec{v}}{\partial t} + (\vec{v} \cdot \nabla) \vec{v} = -\frac{1}{\rho} \nabla \vec{P} + \mu \nabla^2 \vec{v} + \vec{g}[1 - \alpha(T - T_m)]g[1 - \alpha(T - T_m)]. \quad (2)$$

$$\frac{\partial h}{\partial t} + (\vec{v} \cdot \nabla) h = \frac{1}{\rho} (\nabla \cdot k \nabla T) \quad (3)$$

where v is the velocity profile, $\vec{P}$ is pressure, μ is viscosity, $\vec{g}$ is gravity function, α denotes the coefficient of thermal expansion, ρ denotes density, h denotes specific enthalpy, and k is heat conductivity. Following on, the free surface is used to acquire the volume of fluid (VOF) model [27]. We can describe the VOF method as:

$$\frac{\partial V_F}{\partial t} + \nabla \cdot (\vec{v} \cdot V_F) = 0. \quad (4)$$

In Equation (4), V_F denotes the metal volume fraction inside the cell. If $V_F = 1$, it shows that the cell is fully fluid, while $V_F = 0$ indicates that the cell is free of the fluid. Quantities show the existence of a free surface throughout this cell in the center. The differences in the melt pool can be due to several variables, including thermophysical properties, vapor suppression, and/or penetration. The Rosenthal method is extracted from the heat equation, which ignores evaporation, convection, and the Marangoni impact. The corresponding term in Equation (5) for the melt pool diameter extracted from Rosenthal formula is used to describe the role of thermophysical properties in melt pool heterogeneity and the difference in the conduction of heat as:

$$\omega = \sqrt{\frac{8}{\pi e} \cdot \frac{P \eta \eta^n}{\rho C_p V (T_m - T_0)}}, \quad (5)$$

where ω is the melt pool width, P denotes beam power, η is absorptivity, ρ is density, C_p denotes heat capacity, V represents scanning velocity, T_m denotes the melting point, and T_0 denotes the pre-heating level. The Rosenthal solution is obtained under the presumption of thermally independent physical properties, and the thermophysical conductivity is used to measure the melt pool size. The effects of recoil pressure and vapor suppression in the melt pool scale are also incorporated. Each recoil pressure could be calculated by Equation (6):

$$P_S = A \cdot \exp \left\{ B \left(1 - \frac{T_V}{T} \right) \right\}. \quad (6)$$

$$A = \beta P_0, \text{ where } \beta \in [0.54, 0.56]. \quad (7)$$

where P_0 is the atmospheric pressure. The secondary coefficient B is calculated as:

$$B = \Delta H_v / RT_v. \quad (8)$$

In Equation (8), ΔH_v is the accumulated heat of vaporization, R is the gas constant, and T_v is the saturation temperature. The energy density of the beam is known to have a “Gaussian” distribution. During scanning, the beam travels at a constant speed, and the energy density (q) of the beam is expressed as:

$$q = \frac{2Ap}{\pi R_b^2} \exp \left[-2 \frac{(x - vt - x_0)^2 + (y - y_0)^2}{R_b^2} \right]. \quad (9)$$

where A denotes the laser beam absorption coefficient by the powder particles, p represents laser power, R_b indicates the radius of the incident laser beam (spot), v is the rate of scanning, and x_0 and y_0 are the laser beam center's initial location. Convection and radiation were resolved upon this free surface, but evaporation cannot be ignored with the molten pool's surface. As a result, the energy equation, mainly on the surface of the molten pool, may be expressed as:

$$\frac{\partial T}{\partial n} = q - h_c (T^1 - T_0^1) - \sigma_0 \varepsilon (T^4 - T_0^4) - q_{evap}. \quad (10)$$

where h_c is the coefficient of convective heat transfer, T_0 is the room temperature, the Stefan–Boltzmann constant is defined by σ_0 , and ε is a measure of emissivity. Furthermore, q_{evap} is the heat transfer due to evaporation, and can be expressed as:

$$q_{evap} = \omega_0 L_v = \exp(2.52 + 6.121 - 18836T - 0.5 \log T) L_v. \quad (11)$$

where ω_0 is the evaporation rate. For mass flow rate calculation, the following Equation can be used:

$$\dot{m} = \int \rho \cdot \vec{v} d\vec{A}. \quad (12)$$

2.2. LMD Experiments

To validate the developed simulation model, single tracks of AISI 304 stainless steel powder particles were deposited on AISI 304 stainless steel substrate samples via LMD equipment (KR30HA, Kuka, Germany) equipped with a Yb:YAG laser source generating a continuous laser beam ($\lambda = 1030$ nm). The shape of the focused spot is “top-hat” with an 800 μm spot size. The laser scan speed, powder feed rate, and laser power were changed to identify the effects of primary operating conditions on the layer's width and height. The substrate's dimensions were 100 mm $\times$ 100 mm $\times$ 10 mm (L $\times$ H $\times$ W), while the powder particles had 45~106 μm size distribution. Table 2 shows the operating conditions used to perform a total of nine experiments.

Table 2. LMD experimental conditions used to deposit AISI 304 stainless steel powder particles on AISI 304 substrate.

Sample. No.	Laser Power (W)	Laser Scanning Speed (m/s)	Powder Feeding Rate (g/min)	Helium and Argon Gases (bar)	No. of Deposited Tracks	Height/Width of the Clad (mm)
01	700	0.005	3.0	3.0/7.0	1.0	0.42/2.41
02	700	0.015	3.0			0.38/2.12
03	700	0.025	3.0			0.32/1.94
04	500	0.005	2.0			0.10/1.42
05	500	0.005	3.0			0.15/1.59
06	500	0.005	5.0			0.19/1.74
07	500	0.015	5.0			0.47/2.68
08	700	0.015	5.0			0.58/2.97
09	900	0.015	5.0			0.64/3.15

Figure 3 shows the typical cross-section of the typical clad achieved after LMD experiments. The height and width of the deposited layers were used to validate the simulation model.

Figure 3. Cross-section of the clad achieved after LMD experiments.

To analyze the cross-section, metallography steps were applied, as compiled in Table 3.

Table 3. Steps for the grinding and polishing of AISI304 stainless steel.

Name of Step	Item Used for Processing	The Fluid Used for Sample Processing	Revolution/min	Applied Load (N)	Time
Grinding	Silicon carbide paper P320	Water	250	28	Until plane
Polishing	<ul style="list-style-type: none"> Alpha Gamma Lamda 	<ul style="list-style-type: none"> Solution (9.0 μm with diamond) 	<ul style="list-style-type: none"> 150 	<ul style="list-style-type: none"> 24 	<ul style="list-style-type: none"> 5.0
		<ul style="list-style-type: none"> Solution (3 μm with diamond) 	<ul style="list-style-type: none"> 150 	<ul style="list-style-type: none"> 24 	<ul style="list-style-type: none"> 5.0
		<ul style="list-style-type: none"> Solution (0.06 μm with diamond) 	<ul style="list-style-type: none"> 150 	<ul style="list-style-type: none"> 18 	<ul style="list-style-type: none"> 2.0 (water for 30 sec at the end)
Etching	Reagent (V2A)	N/A	N/A	N/A	25 s

3. Results and Discussion

In laser-additive manufacturing processes, generally, two types of melt flow patterns can be identified: (a) conduction mode, and (b) depression mode [28,29]. In the first category, the material is heated at the top, and the laser energy utilized surpasses the proportion at which the heat moves away; the temperature ultimately reaches the melting point, resulting in melt pool formation. For the second category, the laser energy provided by the heating source becomes highly concentrated, so that the material's temperature not only exceeds the melting point, but achieves the boiling point. The rigorous vaporization of the material implies a recoil pressure in the melt pool, resulting in a depression regime. The "depression mode" melt flow is commonly known as "keyhole formation." In depression mode, the heat source melts the outer surface and the inner side of a material. In the present study, only conduction-mode melt flow was identified. The melt pool, with clearly marked boundaries, under "conduction mode" is displayed in Figure 4a–d. The simulations were carried out for the deposition of AISI 304 stainless steel powder particles on AISI 304 stainless steel substrate with a laser power = 900 W, laser scanning speed = 0.015 m/s, and powder flow rate = 5.0 g/min. The stream traces within the melt flow are shown using a solid black line along with the molten material at various time intervals. Through simulations, we found that the melt flow usually adopts a clockwise vortex in front of the laser beam, and an anti-clockwise vortex behind the laser beam. The melt flow along the sidewalls travels from the top to the bottom of the melt pool. During the deposition

process, the bubbles within the melt pool float at a certain velocity and escape from the melt pool. The pores are usually entrapped within the melt pool if the solid front hits the bubble before escaping the melt pool. From the figures, it is clear that the counters of the deposited layer take the longest time for solidification compared to the whole deposition. The bubbles try to escape from the contours, as the liquid region is still present (Figure 4c) at this location. When the material at counters is solidified, the tremendous quantity of bubbles having traveled from different regions to this location due to it having the highest solidification time causes the highest percentage of porosity to be confined to this region. These findings were reported in [30]; however, the real cause was not identified.

Figure 4. Stream traces and solid–liquid transformation during the layer deposition when time is: (a) 0.03 s, (b) 0.08 s, (c) 0.15 s, and (d) 0.20 s.

Figure 5a–d present the top view of the stream traces and solid–liquid transformation during the layer deposition at 0.03 s, 0.08 s, 0.15 s, and 0.20 s time intervals, respectively. The Marangoni flow explained in Figure 4 can be identified clearly. The melt flow adopted a clockwise vortex in the front of the laser beam, while an anti-clockwise vortex was observed behind the laser beam.

To counter-verify the findings described in Figure 4, the stream traces within the melt flow were plotted in Figure 6a–c at 0.08 s, 0.12 s, and 0.16 s, respectively. It can be seen that the melt flow usually adopts a clockwise vortex in front of the laser beam, and an anti-clockwise vortex behind the laser beam.

Figure 7a,b show a comparison between experiments and simulations (approximated values) in terms of layer height and width. The simulation model presented results close to the experimental ones, except for a 1–3% mean absolute deviation. A significantly lower error value proves the reliability of the developed computational fluid dynamics model for the LMD process.

Figure 5. Top view of stream traces and solid–liquid transformation during the layer deposition when time is: (a) 0.03 s, (b) 0.08 s, (c) 0.15 s, and (d) 0.20 s.

Table 4 summarizes the height, width, and grain types provided in Figure 7.

Table 4. Height, width, and grain types for nine AISI 304 stainless steel samples.

Sample No.	Height (mm)		Width (mm)	
	Experiments	Simulations	Experiments	Simulations
01	0.42	0.43	2.41	2.61
02	0.38	0.37	2.12	2.1
03	0.32	0.35	1.94	1.95
04	0.1	0.12	1.42	1.44
05	0.15	0.13	1.59	1.64
06	0.19	0.18	1.74	1.77
07	0.47	0.5	2.68	2.69
08	0.58	0.59	2.97	3
09	0.64	0.66	3.15	3.11

Figure 6. The direction of stream traces within the melt flow when time is: (a) 0.08 s, (b) 0.12 s, and (c) 0.16 s.

Figure 7. Comparison between experimental and simulation (a) height and (b) width in LMD.

The generated melt pool states at (a) 0, (b) 0.12, (c) 0.15, (d) 0.28, (e) 0.31, and (f) 0.35 sec, along with the deposited material's cooling from the melting to room temperature, are displayed in Figure 8a–f. It can be seen that as the temperature increases, the material's density declines quickly, owing to the material's specific heat and latent heat of fusion, thus increasing the fluid volume. These results are consistent with those found in [31,32]. It is worth mentioning that the volume increases drastically due to a decrease in density, which decreases the surface tension (ST). Here, ST is associated with the concentration and thermal gradient, also known as thermocapillary or Benard–Marangoni convection. The difference in ST plays an important role in defining the melt pool. For a given liquid, when the ST difference is developed between the two ends, a strong pull force is formed from the

high ST end to the low ST end. From the figures, it can be seen that when the material was deposited at the substrate, the heat started dissipating from the middle of the deposited layer to the top of the layer and the substrate. The heat traveled from the top of the layer towards the contours or the junction region, resulting in the entire layer's solidification.

Figure 8. Density evolution of the deposited material when time is equal to: (a) 0 s, (b) 0.12 s, (c) 0.15 s, (d) 0.28 s, (e) 0.31 s, and (f) 0.35 s.

Within the melt flow, five major driving forces were identified. “Thermocapillary or Benard–Marangoni convection” causes the material to flow from an elevated to a low thermal regime for a material with a negative thermal surface tension coefficient [33–35]. “Vaporization”-induced recoil pressure applies an internal compression perpendicular to the surface being vaporized [36,37]. “High-speed vapor cloud” can yield shear force via friction at the gas–liquid periphery [38]. “Hydraulic pressure” can transfer energy via either hydrostatic or hydrodynamic pressure [39]. “Buoyancy force” compels the melted material to drive along with the density gradient [39–41]. In the LMD, “thermocapillary or Benard–Marangoni convection” was identified, but it is not dominant in comparison to the selective laser melting (SLM) process [42]. Figure 9a–d show the melt flow pattern with solid–liquid transformation during material deposition. In LMD, the laser beam is responsible for generating a melt pool in the substrate, and for melting down the powder particles added simultaneously along with the laser beam. Let us consider the generated melt pool within the substrate as a “ditch”, which already has molten material. The material deposited earlier will try to enter the melt pool due to the surface gradient, thus affecting the thermocapillary or Benard–Marangoni convection flow generated within the melt pool. The melted powder material being simultaneously added within the melt pool will fill up the “ditch”, causing the overflow of the molten material.

Figure 9. Melt flow pattern of the deposited material when time is equal to: (a) 0.03 s, (b) 0.08 s, (c) 0.15 s, and (d) 0.20 s.

Figure 10a–d compile the cross-sections of the liquid–solid transformation after the layer deposition at various time intervals: (a) 0.24 s, (b) 0.28 s, (c) 0.31 s, and (d) 0.35 s, respectively. It can be seen that when the material is deposited, the heat from the material travels away via conduction, convection, and radiation. The conduction happens by the metal–metal heat exchange, as shown by the thermal isotherms in Figure 10a. Since all of the simulations were conducted at room temperature, the material solidification can be found at the outermost section of the printed layer due to convection and radiation processes. From Figure 10b, three regions can be identified: (a) the melt region, (b) the mushy zone, and (c) the solidified region. The melt region and the mushy zone play important roles in defining a manufactured part’s microstructural evolution and mechanical and physical properties. As time increases, the deposited material’s heat continues to deplete, resulting in layer solidification. These results can be analyzed in Figure 10c,d.

Figure 10. Cross-sections of the liquid-to-solid transformation after the layer is deposited when time is: (a) 0.24 s, (b) 0.28 s, (c) 0.31 s, and (d) 0.35 s.

To analyze the velocity vectors in the melt flow, cross-sections of the deposited layer were taken at different time intervals: (a) 0.03 s, (b) 0.28 s, (c) 0.31 s, and (d) 0.35 s. These results are shown in Figure 11a–d, where the color gradient is present to differentiate the density of the melt pool. In these graphics, the complexity of the melt flow can easily be identified. As explained above, when the laser beam initiates the substrate's irradiation, along with the simultaneous feeding of the powder particles, the melt flow is compelled to flow backward owing to the recoil pressure and thermocapillary or Benard–Marangoni convection effect, as shown in Figure 11a. A reaction force is caused by the velocity vectors at laser–surface periphery. As the laser beam travels, the uppermost region, which is in direct contact with the air, begins to cool, resulting in a drastic increase in the surface tension. Here, it can be seen that the velocity vectors at the top of the surface are dragging the liquid upwards in Figure 11b–d. When the laser beam travels ahead, the flow is pulled by elevated surface tension, as shown in Figure 11b, thus generating a “circular” pattern. The pull force toward the rear end, along with the circular flow pattern, keep increasing, as shown in Figure 11c,d. As time passes, these velocity vectors disappear due to material cooling from the melting to room temperature.

Figure 11. Deposited layer cross-sections of the liquid–solid transformation, with velocity vectors, when time is: (a) 0.03 s, (b) 0.08 s, (c) 0.12 s, and (d) 0.15 s.

Figure 12a–d show the side view of the velocity vectors within the melt flow along with the liquid–solid transformation at 0.03 s, 0.08 s, 0.12 s, and 0.15 s, respectively. The demonstration for these figures is the same as for Figure 11.

Figure 12. Deposited layer side view of the liquid–solid transformation, with velocity vectors, when time is: (a) 0.03 s, (b) 0.08 s, (c) 0.12 s, and (d) 0.15 s.

Figure 13a–d compile the evolution of thermal distribution and the stream traces while printing the AISI 304 stainless steel layer on the AISI 304 stainless steel substrate. During printing, a maximum temperature of 1370 °C was attained—close to the melting point of AISI 304 stainless steel. When the layer is deposited onto the substrate, the deposited material starts to cool down from melting point to room temperature due to the heat losses at the periphery between the layer and the substrate. The outmost layer region is in direct contact with air (Figure 13c). The heat dissipation continues until a solidified layer is achieved, as shown in Figure 13d.

Figure 13. Thermal distribution and stream traces within the deposited layer when time is: (a) 0.03 s, (b) 0.12 s, (c) 0.20 s, and (d) 0.35 s.

Figure 14 shows the mass flow rate calculated for the metal flowing forward and backward, along with the layer's deposition; it shows the behavior of the melt pool flow during and after the laser irradiation. The positive mass flow rate indicates that the flow

is going forward, while the negative shows the flow in the backward direction. At a particular point, after the laser irradiation, the melt pool flows forward. As the laser moves forward from the irradiated region, the melt pool is pulled back due to the difference in the surface tension.

Figure 14. Calculation of the direction of the mass flow rate in the AISI 304 stainless steel deposition via the LMD process.

4. Conclusions

This study developed a computational model for the LMD process by considering the volume of fluid (VOF) and discrete element modeling techniques. A method to track the flow behavior across the entire melt pool was devised. The flow behavior of the melt pool was exposed. Moreover, the driving factors of the liquid flow and fundamental processes were investigated. Furthermore, the deposited layers' height and width were compared with experimental results. A close correlation was determined between the experiments and the simulations, with a deviation of 1–3%. The following conclusions can be reached based on the present study:

- The LMD deposition process involves the simultaneous addition of powder particles. A significant portion of the laser beam energy is utilized by the powder particles to transform their phase from solid to liquid. This, in turn, reduces the net amount of laser energy arriving at the substrate, thus yielding only the conduction-mode melt flow;
- During the deposition process, the bubbles within the melt pool float at a certain velocity and escape from the melt pool. The pores are usually entrapped within the melt pool if the solid front hits the bubble before escaping the melt pool. From simulations, it is clear that the counters of the deposited layer took the longest time to solidify compared to the entire deposition. The bubbles try to escape from the contours and become stuck during solidification, resulting in a tremendous amount of pore formation;
- The positive and negative mass flow rates were identified during the deposition process. The positive mass flow rate shows that the flow is going forward, while the negative shows the flow in the backward direction. When the laser beam heats the material at a specific location, the melt pool flows forward, but as the laser moves forward, the melt pool is pulled back due to the difference in the surface tension. A combination of positive and negative mass flow rates produces discontinuity in the melt pool, which disturbs the microstructural homogeneity in the deposited layer, thus affecting the final thermomechanical characteristics of the printed part. A melt pool can be classified into three regions: (a) a melt region, (b) a mushy zone,

and (c) a solidified region. The mushy zone plays a critical role in defining the microstructural distribution;

- In the LMD, the “thermocapillary or Benard–Marangoni convection” is not dominant compared to the selective laser melting process. The laser beam generates a melt pool in the substrate and melts the powder particles added simultaneously, disturbing the “thermocapillary or Benard–Marangoni convection force” developed in the substrate.

This study provides a cost- and time-effective technique to identify the melt flow and its pattern during the LMD process in detail.

Author Contributions: Conceptualization, methodology, A.U.R. and M.A.M.; formal analysis, A.U.R., M.A.M., F.P. and M.U.S.; investigation, A.U.R., M.A.M., A.C.P. and I.N.M.; writing—original draft preparation, A.U.R. and M.A.M.; writing—review and editing, A.U.R., M.A.M., F.P., M.U.S., A.C.P. and I.N.M.; supervision, F.P., M.U.S., A.C.P. and I.N.M.; project administration, F.P., M.U.S., A.C.P. and I.N.M.; resources, funding acquisition, F.P., M.U.S., A.C.P. and I.N.M. All authors have read and agreed to the published version of the manuscript.

Funding: A.U.R. and M.A.M. have received financial support from the European Union’s Horizon 2020 (H2020) research and innovation program under the Marie Skłodowska-Curie grant agreement No. 764935. A.C.P. has received funding from the PCE57/2021 and PED514/2020 projects, and the Romanian Ministry of Education and Research, under Romanian National Nucleu Program LAPLAS VI—contract no. 16N/2019. A.C.P. and I.N.M. gratefully acknowledge the partial financial support of this work under the POC-G Contract no. 135/2016. This project has received funding from the European Union’s Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 764935. The generous support is gratefully acknowledged.

Data Availability Statement: Not applicable.

Acknowledgments: The authors acknowledge with thanks the support of European Union’s Horizon 2020 (H2020) research and innovation program, Romanian Ministry of Education and Research and the Turkish Aerospace for the CFD post processing.

Conflicts of Interest: The authors declare no conflict of interest.

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