

Multi-phase semi-resolved CFD-DEM for high-fidelity modeling of powder-based directed energy deposition

Tao Yu^{a,b,*}, Yong Kong^{b,c}, Jidong Zhao^{b,**}

^a State Key Laboratory of Soil Pollution Control and Safety, Zhejiang University, Hangzhou, China

^b The Hong Kong University of Science and Technology, Clearwater Bay, Kowloon, Hong Kong Special Administrative Region of China

^c Chengdu University of Technology, State Key Laboratory of Geohazard Prevention and Geoenvironment Protection, Chengdu, China

ARTICLE INFO

Keywords:

Coupled CFD-DEM
Multiphase flow dynamics
Directed energy deposition
Additive manufacturing
Ray-tracing
Melt pool dynamics

ABSTRACT

Powder-based directed energy deposition (PB-DED) has emerged as a promising additive manufacturing technology for large-scale metal components, yet its process fidelity is plagued by the complex interplay of particle-laden flow, laser energy distribution, and melt track hydrodynamics. To overcome limitations of existing models that oversimplify these multi-physics phenomena, this study presents a high-fidelity, multi-phase computational framework based on a semi-resolved Computational Fluid Dynamics and Discrete Element Method (CFD-DEM) coupling. The framework integrates (i) a kernel-based semi-resolved CFD-DEM coupling algorithm for accurate particle-fluid momentum and heat exchange; (ii) a temperature-dependent multiphase Volume-of-Fluid (VOF) method capturing melting, solidification, and dynamic wetting via a generalized contact angle model and a phase-transition model; (iii) a conjugate heat transfer formulation enabling bidirectional thermal coupling between particles, melt pool, and substrate; and (iv) a ray-tracing laser model that resolves multiple reflections and energy absorption across both discrete particles and the diffuse melt pool surface. The framework is rigorously validated against four benchmark cases, demonstrating exceptional accuracy in predicting powder stream focusing, laser-particle interaction, melt pool dynamics, contact-angle-dependent wetting, and final melt track morphology. Beyond quantitative validation, the simulations provide mechanistic explanations for PB-DED defects, including the balling effect and discontinuous interfaces. Leveraging full-process GPU acceleration, the framework enables large-scale simulations of multi-laser, multi-powder-stream PB-DED on standard desktop hardware, achieving unprecedented computational efficiency and scalability. This work establishes a robust, predictive computational platform for defect analysis, process optimization, and digital twin development in metal additive manufacturing.

1. Introduction

Powder-based directed energy deposition (PB-DED) has emerged as a versatile metal additive manufacturing (AM) technology, distinguished by its capability for large-scale component fabrication, high-value part repair, and the production of functionally graded materials [1]. Unlike laser powder bed fusion (LPBF), PB-DED offers superior deposition rates, greater flexibility in material feedstock, and compatibility with multi-axis robotic systems [2,3], making it particularly suitable for industrial applications in aerospace [4,5], infrastructure [6,7], and medical implants [8,9], where customization [5], lead-time reduction [10], and material efficiency [11] are critical. However, the industrial

adoption of PB-DED is hampered by its inherent complexity. The process involves highly coupled multi-physics phenomena [12,13], including powder-gas flow, laser-particle interaction, melt pool dynamics, and thermal-induced phase changes, that collectively govern deposition quality, microstructural evolution, and the formation of defects such as porosity and balling [14,15]. Achieving a predictive understanding of these interactions is essential for robust process control and represents a fundamental challenge in the field [2].

Substantial experimental efforts have been directed at addressing this challenge [16,17]. *In-situ* monitoring techniques, including coaxial optical imaging, thermography, and pyrometry, have been employed to capture melt pool characteristics and enable closed-loop control

* Corresponding author at: State Key Laboratory of Soil Pollution Control and Safety, Zhejiang University, Hangzhou, China.

** Corresponding author.

E-mail addresses: tyuak@connect.ust.hk (T. Yu), jzhao@ust.hk (J. Zhao).

<https://doi.org/10.1016/j.addma.2026.105288>

Received 9 January 2026; Received in revised form 1 May 2026; Accepted 1 July 2026

Available online 3 July 2026

2214-8604/© 2026 Elsevier B.V. All rights are reserved, including those for text and data mining, AI training, and similar technologies.

[18–20]. Complementary approaches using acoustic emission (AE) sensors and microphones offer cost-effective detection of anomalies [2, 21–23], while high-speed X-ray imaging provides unparalleled, direct observation of subsurface phenomena such as pore formation and migration [24,25]. Despite its success in LPBF [26,27], the application of such high-fidelity diagnostics to PB-DED remains limited [28]. Furthermore, although machine learning has shown promise in analyzing monitoring data for defect detection and classification accuracy [29–31], these data-driven methods often lack generalizability and the fundamental physical insights needed for predictive modeling across diverse materials and processing conditions.

Despite these advances, experimental approaches remain costly, time-consuming, and challenging to scale to production environments. Critically, they offer limited access to transient, three-dimensional internal physical fields, such as local velocity, pressure, and temperature distributions within the melt pool, which are essential for understanding the root cause of defect formation. While data-driven methods show promise, they often struggle with robustness and generalizability across different alloys, process conditions, and machine platforms. These limitations underscore the necessity for high-fidelity, physics-based numerical models that can complement experiments by providing detailed spatial-temporal insights, thereby enabling systematic process optimization and the design of reliable monitoring and control strategies.

To complement experimental efforts, a range of computational models have been developed for PB-DED, though they remain less extensive than those for LPBF [28,32]. Existing approaches can be broadly categorized as finite element method (FEM)-based [33–35], computational fluid dynamics (CFD)-based [28, 36–39], or discrete element method (DEM)-based [40]. FEM-based models excel at predicting part-scale thermo-mechanical responses, such as residual stress, distortion, and large-scale thermal histories [38,40]. In many of these studies, deposition is modeled using an Arbitrary Lagrangian-Eulerian (ALE) formulation, where the addition of powder material is represented through an equivalent mass source [41,42]. This strategy allows the evolving deposition surface and geometric features, including overall bead shape and surface roughness trends, to be approximated efficiently at the macroscopic scale. However, because the powder stream is typically treated as a continuum mass input, the underlying discrete powder dynamics, laser-particle interactions, and particle-scale thermal heterogeneity cannot be resolved explicitly.

In contrast, CFD-based studies offer a more direct representation of melt pool hydrodynamics and free-surface evolution, enabling higher-fidelity tracking of defect formation mechanisms [43]. These models have been successfully applied to investigate the influence of process parameters such as laser power, scan speed [37], powder feed rate [36], external fields [38], and multi-material deposition [39]. However, the predictive capability of most existing CFD models is constrained by considerable simplifications of the underlying physics [28, 36–39, 44, 45]. Key mechanisms frequently neglected include the complex multiple reflections of the laser within the powder stream and at the melt pool surface, the resolved dynamics and temperature heterogeneity of individual powder particles, and the fully coupled interactions among the shielding gas, powder particles, and the evolving melt track.

More recently, CFD-DEM approaches have been introduced to better describe the behavior of discrete powder particles. However, existing studies often focus on individual subprocesses rather than the entire PB-DED chain. For example, some CFD-DEM models employ two-way coupling to simulate powder stream dynamics, capturing the interaction between carrier gas flow and particle trajectories [46,47], but they usually neglect particle melting. Conversely, other studies based on one-way coupling investigate laser-particle heating and melting [48–50], but often simplify particle motion using DEM alone, without fully resolving the fluid-particle coupling. More recent efforts [51–53] have extended the CFD-DEM framework by incorporating hydrodynamic forces acting on particles, as well as the critical impact of powder-induced attenuation on laser power and intensity profiles and

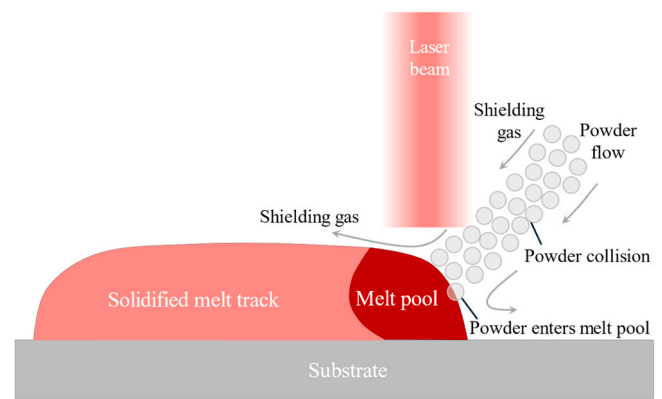


Fig. 1. Schematic illustration of the powder-based directed energy deposition (PB-DED) process, showing powder injection, laser irradiation, melt pool formation, and solidified track.

the influence of beam shaping on solidification microstructure evolution, thereby advancing the physical fidelity of the models. However, these approaches still lack a fully consistent two-way coupling scheme and high-fidelity laser ray-tracing models. As a result, these models are still insufficient to simulate the full PB-DED process in a unified, fully coupled manner. Key physical interactions across the powder stream, laser energy absorption, and melt pool evolution cannot be captured simultaneously, limiting predictive accuracy for practical manufacturing scenarios. Furthermore, the computational scale of these simulations is typically small [50,53], often limited to single-track or single-powder-stream cases, far from representing realistic multi-track, multi-layer deposition. For instance, a representative simulation with approximately 4.7×10^8 computational cells may require on the order of four days on a 16-core CPU platform [51], highlighting the prohibitive computational cost. Such efficiency limitations significantly hinder the extension of these approaches to component-scale manufacturing simulations.

To bridge this gap, we propose a novel multi-phase, semi-resolved CFD-DEM framework for high-fidelity and computationally efficient simulation of PB-DED processes (Fig. 1). The main contributions of this work are threefold. First, an existing semi-resolved CFD-DEM framework is adapted and extended for PB-DED processes by incorporating problem-specific physical models, including particle collision dynamics and phase change behavior, together with a ray-tracing-based laser model tailored for metal powder and melt pool interactions, enabling consistent coupling among particles, fluid, and laser energy deposition. Second, the algorithms are redesigned and optimized for GPU architectures to fully exploit parallelism, and are further applied to simulate multi-track, multi-laser, and multi-layer deposition processes, bridging high-fidelity modeling toward realistic manufacturing scenarios. Third, the model is employed to systematically investigate the underlying mechanisms of balling effect, as well as the formation of discontinuous interfaces induced by bifurcating paths in multi-track, multi-layer deposition.

Our approach strategically resolves the problem across its constituent scales: the melt pool and gas phases are treated as continua, while powder particles are explicitly modeled using DEM to capture their kinematic and thermal evolution. A kernel-based approximation is employed to rigorously evaluate the interphase momentum and heat exchange among powder, gas, and the melt track. Crucially, laser energy deposition is modeled using a spatially resolved ray-tracing approach that accounts for multiple reflections, ensuring physically consistent energy absorption by both powders and fluids. The integrated framework enables the coupled simulation of powder injection, laser-particle interaction, melt pool dynamics, thermal field evolution, and thermally induced phase transformations under realistic processing conditions. It therefore provides a robust and versatile computational tool for

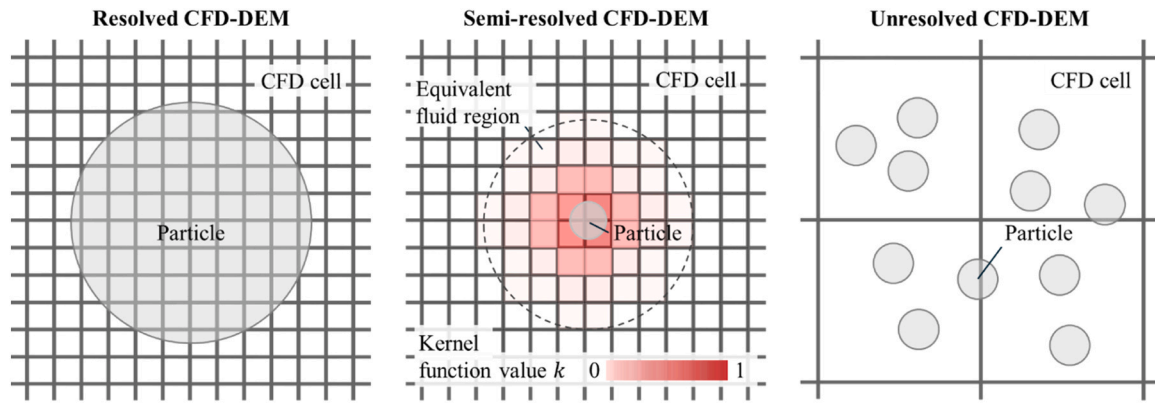


Fig. 2. Schematic of the three coupled CFD-DEM regimes classified by grid-to-particle size ratio, shown from left to right as resolved, semi-resolved, and unresolved approaches.

elucidating defect formation mechanisms and supporting the design and optimization of industrial PB-DED processes. The nomenclature used in this paper is provided in Table A.1.

The entire framework is fully GPU-accelerated to ensure high computational efficiency and scalability. All computational modules (except input and output operations) are rewritten in CUDA C++ and executed directly on the GPU. The traditional CPU-based domain-decomposition parallel strategy is replaced by a fine-grained thread-level parallelization scheme [54], in which computational tasks are mapped to mesh cells and faces. Key components, including equation assembly, the laser ray-tracing module, and the particle-fluid coupling and conversion procedures, have been redesigned using dedicated GPU-oriented algorithms to maximize parallel efficiency while minimizing memory-transfer overhead. For representative additive manufacturing simulations (e.g., LPBF cases), the proposed fully GPU-resident framework achieves approximately a $20 \times$ speedup compared with conventional CPU-based implementations [55]. In a representative multi-laser, multi-track, and multi-layer PB-DED case, employing adaptive mesh refinement with an average grid size of approximately 1.7 million cells, the simulation can be completed within about 9 h on a cost-effective RTX 5070 GPU, demonstrating its practical capability for complex, large-scale process modeling.

2. Methodology: multi-phase semi-resolved CFD-DEM framework for PB-DED

2.1. Multiphysics modeling of gas-melt pool-powder coupled flow

2.1.1. Numerical considerations for semi-resolved CFD-DEM modelling of PB-DED

Coupled CFD-DEM methods are commonly classified according to mesh resolution versus particle size into resolved, semi-resolved, and unresolved schemes (Fig. 2), corresponding to mesh-to-particle diameter ratios typically $< 1/3$, ≈ 1 , and > 8 , respectively [56]. While we previously employed a resolved CFD-DEM approach for LPBF simulations [32], a semi-resolved scheme is adopted here for PB-DED due to a fundamental difference in process scale between PB-DED and LPBF. The distinguishing factor lies in relative scale of the process zone (melt track or laser spot) to the powder particles. In LPBF, the melt pool and laser spot are only a few times larger than the particle diameter, necessitating high-resolution, particle-resolved modeling. In contrast, the melt track in PB-DED can be several tens of times larger than the individual powder particles, enabling a much higher deposition rate and making it suitable for large-scale component fabrication [2,3]. This scale disparity motivates the use of a semi-resolved CFD-DEM approach for PB-DED based on balanced consideration of the following two aspects:

- (1) **Computational accuracy:** The influence of partially melted particles on the final melt-track morphology is negligible in PB-DED, where the particle diameter is typically less than 4% of the melt-track width (or laser spot size). This is due to three factors: (i) the Gaussian laser profile distributes energy more uniformly over the larger process zone, suppressing intense localized heating of individual particles; (ii) any partial melting only marginally increases surface roughness relative to the overall track dimensions; and (iii) as PB-DED operates predominantly in conduction mode [28], particles entering the melt pool are rapidly assimilated and fully melted. While this simplification neglects localized thermal and momentum effects from particle impact, our validation (Section 3.4) confirms that the net effect on final morphology falls within experimental error. Therefore, resolving the bulk melt pool thermodynamics is sufficient. Our simulations maintain high fidelity by resolving the melt track width with over 25 cells, a resolution comparable to resolved CFD-DEM in LPBF.
- (2) **Computational efficiency:** The computational cost of a resolved CFD-DEM approach for PB-DED would be prohibitive, estimated to be several hundred times higher than the semi-resolved method [56]. To illustrate, employing an LPBF-level resolution (mesh size = $1/8$ particle diameter) for a representative PB-DED track would require $\sim 10^8$ cells, as the mesh would need to resolve features $1/200$ th of the melt track width. This is impractical for engineering applications. In contrast, the semi-resolved approach, with a mesh size on the order of the particle diameter, reduces the cell count in this example to $\sim 1.95 \times 10^5$. This achieves an optimal balance between accuracy and efficiency, making large-scale simulations feasible.

It should be noted that the present modeling framework primarily focuses on resolving the thermo-fluid dynamics of the coupled powder-laser-melt pool interaction. Consequently, certain metallurgical phenomena, such as microstructure evolution and the potential entrapment of gas porosity between adjacent tracks, are not explicitly considered. The melt track morphology discussed in later sections is therefore interpreted mainly from a thermal perspective, representing the degree of thermal overlap between successive tracks rather than a direct prediction of metallurgical bonding quality. Incorporating microstructure evolution and defect formation mechanisms would require additional physics-based models and will be explored in future work.

2.1.2. Governing equations of CFD and DEM

In this study, the fluid dynamics are solved using a finite-volume-based CFD approach. Within the semi-resolved CFD-DEM framework, the continuity and momentum equations are modified by introducing

the fluid void fraction ε and the particle-fluid interaction force $\mathbf{F}_f$. The formulation of ε and $\mathbf{F}_f$ will be detailed in subsequent sections (Section 2.1.3 and Section 2.1.4). The right-hand side of Eq. (1) incorporates eight distinct terms, representing contributions from pressure, gravity, viscosity, surface tension, particle-fluid interaction, Darcy flow [57,58], Marangoni effect, and recoil pressure, respectively. In this formulation, the fluid velocity corresponds to the interstitial velocity within the pore space. Therefore, the governing equations are expressed in a porosity-weighted form, where the local void fraction accounts for the volume displacement caused by particles within each computational cell. This formulation corresponds to the widely adopted Type A (Model A) framework in CFD-DEM coupling, which has been extensively used in semi-resolved particle-fluid simulations [56,59].

$$\begin{aligned} \frac{\partial}{\partial t}(\varepsilon \rho \mathbf{u}) + \nabla \cdot (\varepsilon \rho \mathbf{u} \otimes \mathbf{u}) = & -\varepsilon \nabla p + \varepsilon \rho \mathbf{g} + \nabla \cdot (\varepsilon \mu \cdot (\nabla \mathbf{u})) + \varepsilon \mathbf{F}_t - \mathbf{F}_f \\ & - \varepsilon K_c \frac{(\alpha_1 - \alpha_m)^2}{\alpha_m^3 + C_k} \mathbf{u} \\ & + \varepsilon \frac{d\sigma}{dT} (\nabla T - \mathbf{n}(\mathbf{n} \cdot \nabla T)) |\nabla \alpha_1| \frac{2\rho}{\rho_{\text{sum}}} \\ & + 0.54 \varepsilon p_0 \exp\left(L_v M \frac{T - T_{LV}}{RTT_{LV}}\right) |\nabla \alpha_1| \frac{2\rho}{\rho_{\text{sum}}} \mathbf{n} \end{aligned} \quad (1)$$

where ρ , $\mathbf{u}$, μ and p represent the density, velocity, viscosity, and pressure of fluid, respectively. The density ρ and viscosity μ represent the equivalent properties of the two-phase mixture, which are defined in Section 2.2.1. $\mathbf{g}$ is the gravitational acceleration. $\mathbf{F}_t$ is calculated as $\mathbf{F}_t = c\sigma |\nabla \alpha_1| \mathbf{n}$, where α_1 is the volume fraction of metal. σ denotes the surface tension coefficient, and c represents the curvature of the fluid-gas interface, defined as $c = -\nabla \cdot \mathbf{n}$, with $\mathbf{n}$ being the unit normal vector at the interface, while on a solid interface, $\mathbf{n}$ is set to $\mathbf{n} = \mathbf{n}_c$, reconstructed according to the specified contact angle. For a free surface, $\mathbf{n}$ is computed as $\mathbf{n} = \nabla \alpha_1 / |\nabla \alpha_1|$. $d\sigma/dT$ represents the temperature derivative of the surface tension coefficient. $\rho_{\text{sum}} = \rho_1 + \rho_2$ denotes the sum of the density of phases at the interface. The term $2\rho/\rho_{\text{sum}}$ acts as a density-weighting factor in the sharp surface force (SSF) formulation, which is introduced to smear out the interface force over a finite thickness and improve numerical stability in the vicinity of the interface [60,61]. K_c denotes the permeability coefficient [62], and $C_k = 10^{-5}$ is a small constant introduced to prevent division by zero. This Darcy-type resistance is applied only within the solidified region and the mushy zone, which corresponds to a narrow temperature interval between the solidus and liquidus temperatures (≈ 45 K for Ti6Al4V and ≈ 30 K for AISI 304). The corresponding validation cases can be found in Ref. [63]. The term α_m represents the volume fraction of molten metal, which can be approximated using a Gaussian error function [64] as $\alpha_m = \frac{\alpha_1}{2} [1 + \text{erf}(\frac{4}{T_1 - T_s}(T - \frac{T_1 + T_s}{2}))]$. T_1 , T_s , and T_{LV} are the liquidus, solidus, and boiling temperatures, respectively. L_v denotes the latent heat of vaporization. M is the molar mass and R is the universal gas constant.

Particle motion is described by the DEM through the linear and angular momentum equations for each individual particle (Eq. (2)). The model accounts for multiple interaction forces [65,66], including particle-particle collision $\mathbf{F}_{p-p}$, particle-wall collision $\mathbf{F}_{p-w}$, and fluid-particle interaction $\mathbf{F}_f$ [67]. The particle properties, such as density and size distribution, are detailed in the model setup section of each subsequent numerical example.

$$\begin{cases} m_p \frac{d\mathbf{v}}{dt} = \mathbf{F}_s + m_p \mathbf{g} + \sum \mathbf{F}_{p-p} + \sum \mathbf{F}_{p-w} \\ \mathbf{I}_p \frac{d\boldsymbol{\omega}}{dt} = \sum \mathbf{M}_t + \sum \mathbf{M}_r \end{cases}, \quad (2)$$

where $\mathbf{v}$ and $\boldsymbol{\omega}$ represent the linear and angular velocities of Particle p ,

respectively. The mass and rotational inertia of Particle p are denoted by m_p and $\mathbf{I}_p$, respectively. $\mathbf{M}_t$ and $\mathbf{M}_r$ correspond to the torque induced by the tangential force and the rolling friction torque [68], respectively. The Hertzian contact law, combined with Coulomb's friction law, is employed to characterize the interparticle contact behavior [69].

The thermal field of the fluid phase is governed by the temperature Eq. (3), derived from the principle of energy conservation. The eight terms on the right-hand side represent, respectively, laser energy input (S_{lf}), heat transfer from particles (S_f), thermal conduction, viscous dissipation, latent heat of fusion, convection, radiation, and vaporization. For the thermal boundary conditions, a simplified treatment is adopted, and no specific thermal resistance or heat transfer coefficient is prescribed at the substrate-fixture interface. This choice follows common practice in previous studies [32,70,71] and is primarily due to the limited availability of reliable experimental data for such parameters.

$$\begin{aligned} \frac{\partial}{\partial t}(\varepsilon C_p T) + \nabla \cdot (\varepsilon C_p \mathbf{u} T) = & S_{lf} + S_f + \nabla \cdot (\varepsilon k \nabla T) + \varepsilon \mu (\nabla \mathbf{u} + \mathbf{u} \nabla) : \nabla \mathbf{u} \\ & - \varepsilon L_f \left[\frac{\partial}{\partial t}(\rho \alpha_m) + \nabla \cdot (\rho \mathbf{u} \alpha_m) \right] \\ & - \varepsilon h_c (T - T_{\text{ref}}) |\nabla \alpha_1| \frac{2C_p}{(C_i \rho_i)_{\text{sum}}} \\ & - \varepsilon C_e \sigma_{\text{sb}} (T^4 - T_{\text{ref}}^4) |\nabla \alpha_1| \frac{2C_p}{(C_i \rho_i)_{\text{sum}}} \\ & - \varepsilon \frac{0.82 p_0 L_v M}{(2\pi MRT)^{0.5}} \exp\left(L_v M \frac{T - T_{LV}}{RTT_{LV}}\right) |\nabla \alpha_1| \frac{2C_p}{(C_i \rho_i)_{\text{sum}}}, \end{aligned} \quad (3)$$

where k is the thermal conductivity of the fluid, L_f is the latent heat of fusion, h_c is the convective heat transfer coefficient, T_{ref} is the reference temperature, C_e is the emissivity of the particle, and σ_{sb} is the Stefan-Boltzmann constant. The term $(C_i \rho_i)_{\text{sum}} = C_1 \rho_1 + C_2 \rho_2$ represents the sum of the products of density ρ and heat capacity C of the phases at the interface.

The particle temperature evolution is described by Eq. (4), accounting for particle-particle heat transfer (S_{p-p}), particle-fluid heat exchange (S_p), and absorbed laser energy (S_{lp}). The final term represents latent heat consumption during melting. As detailed in Section 2.2.2, only particles that have contacted the melt track and exceeded the liquidus temperature undergo phase transition. Before this moment, their temperature may rise to the solidus or even the liquidus point, requiring latent heat to be included:

$$\frac{\partial}{\partial t}(m_p C_p T_p) = S_{lp} + S_p + S_{p-p} - L_f m_p \frac{\partial \alpha_m}{\partial t}, \quad (4)$$

where C_p and T_p denote the heat capacity and temperature of the particle, respectively. The particle-fluid heat transfer term S_p and the laser energy input term S_{lp} will be discussed in detail in the subsequent subsections. S_{p-p} represents the total energy exchanged between a given particle and all surrounding particles, and its calculation formula is given by

$$(S_{p-p})_i = \sum_j \frac{4k_i k_j}{k_i + k_j} \sqrt{A_c} (T_{pj} - T_{pi}), \quad (5)$$

$$A_c = \pi \left[\frac{5m_p^* R^{*2}}{4E^*} (\mathbf{v}_i - \mathbf{v}_j)^2 \right]^{2/5}, \quad (6)$$

where k is the thermal conductivity of the particle. The subscripts i and j denote particle i and particle j , respectively. Σ denotes the population of all particles that interact with particle i through collision. A_c is the contact area between two particles. This area is a function of the effective mass m_p^* and Young's modulus E^* , and radius R^* , which are defined as follows:

$$m_p^* = \frac{m_{pi}m_{pj}}{m_{pi} + m_{pj}}, \quad (7)$$

$$E^* = \frac{4}{3} \left(\frac{1 - v_i^2}{E_i} - \frac{1 - v_j^2}{E_j} \right)^{-1}, \quad (8)$$

$$R^* = \frac{R_i R_j}{R_i + R_j}, \quad (9)$$

2.1.3. Kernel-based approximation method

Following the approach of Wang et al. [56], a kernel-based approximation (Eq. (10)) is employed to reconstruct the void-fraction field and compute the fluid-particle interaction force. In accordance with Wang et al. [56], a Gaussian kernel is adopted with a smoothing distance equal to two particle diameters. The method defines an equivalent fluid region (see middle panel of Fig. 2) with a characteristic length of at least three particle diameters, thereby satisfying the spatial-resolution requirements of the drag model used in unresolved CFD-DEM simulations [72]. In practice, contributions are considered from cells within four particle diameters of particle i where the kernel function value k_{ij} exceeds 0.1, approximately 10% of its maximum value, which occurs when the cell center coincides with the particle center.

$$k_{ij} = e^{-\|C_j - C_i\|^2 / (8d_i^2)}, \quad (10)$$

where k_{ij} represents the value of the kernel function of particle i evaluated at cell j . C_i and C_j denote the centers of particle i and cell j , respectively. $\|C_j - C_i\|$ represents the distance between the center of particle i and the center of cell j . d_i is the diameter of particle i .

The void fraction ε quantifies the fraction of a CFD cell's volume not occupied by particles. In the semi-resolved framework, however, this quantity is evaluated over equivalent regions rather than individual cells, necessitating a kernel-based volume-distribution procedure. The governing equations are given in Eqs. (11) and (12). The overall procedure consists of three steps:

- (1) **Kernel contribution:** For each particle i , the kernel function (Eq. (10)) determines its contribution k_{ij} to every cell j within the equivalent region.
- (2) **Volume distribution:** The contributions are normalized to obtain weights C_{ij} for all affected cells (Eq. (12)). Each particle's volume is then distributed among these cells in proportion to C_{ij} (Eq. (11)).
- (3) **Void fraction field:** After processing all particles, the total particle volume assigned to each cell is obtained. The void fraction of cell j is finally computed as the unoccupied volume fraction relative to the cell volume (Eq. (11)).

$$\varepsilon_j = 1 - \frac{\sum C_{ij} V_{pi}}{V_j}, \quad (11)$$

$$C_{ij} = \frac{k_{ij}}{\sum k_{ik}}, \quad (12)$$

where C_{ij} denotes the normalized weight, i.e., the fraction of the volume of particle i that is assigned to cell j . $\sum C_{ij} V_{pi}$ represents the total particle volume contributed to cell j by all particles within its equivalent region. V_j is the volume of cell j .

2.1.4. Particle-fluid interaction and heat transfer

Unlike unresolved CFD-DEM, where the fluid-particle force is computed directly from the flow variables of the cell containing the particle, the semi-resolved approach reconstructs an equivalent flow

field around the particle using a normalized kernel-based weighting that also accounts for cell volume and local void fraction. The equivalent flow variable [56] is obtained via Eqs. (13) and (14).

$$\bar{\eta} = \sum \eta_j C_{ij}, \quad (13)$$

$$C'_{ij} = \frac{\varepsilon_j V_j k_{ij}}{\sum \varepsilon_k V_k k_{ik}}, \quad (14)$$

where η_j denotes an arbitrary variable of fluid cell j , and the overline indicates its equivalent value. C'_{ij} denotes the normalized weight.

The interaction force exerted on the fluid (F_f) and on the particle (F_s) considers all particle-cell pairs within the equivalent region, thereby incorporating the influence of neighboring particles and cells. In the present study, only the drag force and virtual mass force are considered, following common practices reported in previous studies [51,73].

$$F_{f,j} = \frac{1}{V_j} \sum_{i=1}^n (\mathbf{f}_{d,ij} + \mathbf{f}_{vm,ij}), \quad (15)$$

$$F_{s,i} = \sum_{j=1}^n \left(-V_{pi} (\bar{\nabla} p + \bar{\nabla} \cdot (\mu \cdot (\bar{\nabla} \mathbf{u})))_j + \mathbf{f}_{d,ij} + \mathbf{f}_{vm,ij} \right), \quad (16)$$

where n denotes the number of particle-cell pairs within the equivalent region, and the summation symbol $\sum$ represents the aggregation of the interaction forces. The subscript i refers to particle i , and the subscript j refers to fluid cell j . The first term in the equation for F_s represents the force exerted on the particle by fluid viscosity and pressure difference, with the overline indicating that this term is evaluated as an equivalent value using Eq. (13). The term $\mathbf{f}_d$ denotes the drag force arising from the velocity difference, whereas $\mathbf{f}_{vm}$ represents the virtual mass force induced by the acceleration difference. These two forces are computed as follows [72,74,75]:

$$\mathbf{f}_{d,ij} = \frac{1}{8} C_d \pi \rho_j d_i^2 (\bar{\mathbf{u}}_j - \mathbf{v}_i) |\bar{\mathbf{u}}_j - \mathbf{v}_i| e_j^{1-\chi}, \quad (17)$$

$$\mathbf{f}_{vm,ij} = \left(2.1 - \frac{0.132}{0.12 + A_c^2} \right) \frac{V_{pi} \rho_j}{2} |\bar{\mathbf{u}}_j - \dot{\mathbf{v}}_i|, \quad (18)$$

where $\bar{\mathbf{u}}$ and $\dot{\mathbf{v}}$ represent the accelerations of the fluid and the particles, respectively. The fluid acceleration at the particle location is evaluated from the temporal variation of the interpolated fluid velocity, obtained using the interpolation scheme described in Section 2.1.3. The coefficients C_d , χ , and A_m in Eqs. (17) and (18) are computed as:

$$C_d = \left(0.63 + \frac{4.8}{\sqrt{\text{Re}}} \right)^2, \quad (19)$$

$$\text{Re} = \frac{\varepsilon_j \rho_j d_i}{\mu_j} |\bar{\mathbf{u}}_j - \mathbf{v}_i|, \quad (20)$$

$$\chi = 3.7 - 0.65 \exp \left[-\frac{(1.5 - \log_{10} \text{Re})^2}{2} \right], \quad (21)$$

$$A_m = \frac{\|\bar{\mathbf{u}}_j - \mathbf{v}_i\|^2}{d_i \|\bar{\mathbf{u}}_j - \dot{\mathbf{v}}_i\|}, \quad (22)$$

where C_d denotes the particle-fluid drag coefficient, which is a function of the particle Reynolds number Re . The term $e^{-\chi}$ represents a correction factor that accounts for the influence of neighboring particles on the drag force acting on the particle under consideration.

In the present semi-resolved CFD-DEM framework, the influence of particle rotation on the fluid-particle interaction forces is not explicitly resolved. Hydrodynamic forces are evaluated based on the relative translational velocity between the particle and the surrounding fluid. Resolving the hydrodynamic effects induced by particle rotation would

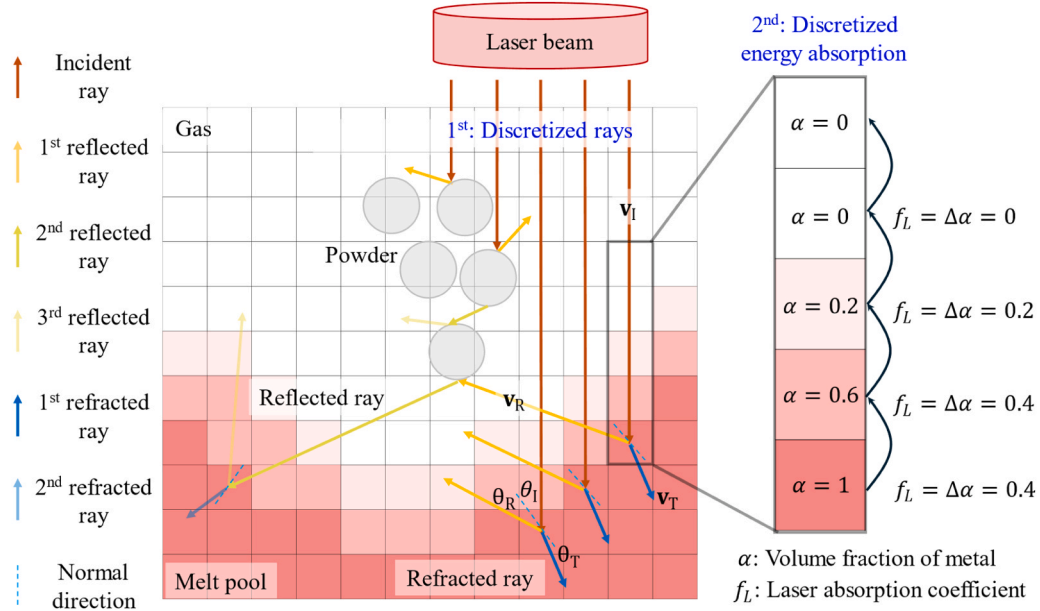


Fig. 3. Schematic diagram for the VOF compatible ray tracing model.

require a fully resolved fluid-particle coupling approach with significantly finer grids around each particle, which would incur prohibitively high computational costs for large-scale simulations considered here. Moreover, in the PB-DED process considered here, the particle diameter is typically much smaller than the characteristic melt-track width, and melt pool dynamics are governed primarily by surface tension and Marangoni convection. Therefore, the influence of particle rotation on the overall fluid flow and melt pool behavior is expected to be limited. In the current model, particle rotation is retained only insofar as it affects contact mechanics between particles through the DEM collision formulation.

The heat source terms S_f and S_p in Eqs. (3) and (4) represent the energy exchange between the particles and the background fluid, which is governed by the particle temperature and the fluid temperature surrounding the particles. The expression for the source term S_f in the temperature equation of CFD is given in Eq. (23). Specifically, in this study, a normalized weight C_{ij} in Eq. (14) is employed in the calculation of S_f to account for all particle-cell pairs within the equivalent region.

$$S_{f,i} = \frac{1}{V} \sum_{j=1}^n C_{ij} S_i \left[h_i (T_{pi} - T_j) + C_e \sigma_{sb} (T_{pi}^4 - T_j^4) \right], \quad (23)$$

where V is the cell volume and $S_i = \pi d_i^2$ denotes the surface area of particle i . Here, n represents the number of particle-cell pairs within the equivalent region, and the summation operator $\sum$ signifies the aggregation of particle-fluid energy transfer. The heat transfer coefficient, h_i is defined as $h_i = Nu_i k / d_i$, where Nu_i is the particle Nusselt number [76]. For Eq. (23), Nu_i is computed individually for each particle-cell pair using the corresponding local cell information. It should be noted that this correlation has been widely used in particle-fluid systems to estimate gas-particle convective heat transfer [56]. In the present DED process, the heating of particles is dominated by laser absorption, while the contribution of gas convection remains comparatively small due to the low thermal conductivity of the shielding gas. This Nusselt number is computed based on the void fraction field ϵ , particle Reynolds number Re , and Prandtl number Pr :

$$Nu_i = \begin{cases} 2 + 0.6 \epsilon^{3.5} Re^{0.5} Pr^{1/3} & Re \leq 200 \\ 2 + \epsilon^{3.5} (0.5 Re^{0.5} + 0.02 Re^{0.8}) Pr^{1/3} & 200 < Re \leq 1500 \\ 2 + 0.00045 \epsilon^{3.5} Re^{1.8} & Re > 1500 \end{cases}, \quad (24)$$

where the Prandtl number Pr characterizes the relative magnitude of momentum diffusivity to thermal diffusivity in a fluid, which is calculated as $Pr = C\mu/k$.

The source term S_p in the DEM temperature equation is given by Eq. (25) and is evaluated using a particle-cell pair-based formulation similar to that in Eq. (23). The key difference lies in that Eq. (23) is cell-centered, whereas Eq. (25) is particle-centered, while ensuring overall energy conservation.

$$S_{p,i} = \sum_{j=1}^n -C_{ij} S_i \left[h_i (T_{pi} - T_j) + C_e \sigma_{sb} (T_{pi}^4 - T_j^4) \right], \quad (25)$$

2.1.5. Ray tracing model for the laser beam in PB-DED

This study introduces an improvement to our previously developed VOF-compatible ray-tracing model [77], originally designed for resolved CFD-DEM, and adapts it for calculating the laser energy absorbed by both particles and fluids. Fig. 3 shows the schematic diagram for the proposed ray tracing model. The improved algorithm offers three major strengths for generating high-resolution laser energy fields: (1) It is capable of accounting for multiple reflections and refractions at the interfaces between particles, the substrate, and the melt track; (2) It is compatible with highly efficient GPU parallel computing by discretizing the continuous laser beam into tens of millions of discrete rays; (3) It can adapt to the diffuse fluid interface captured by the VOF method through distributing the energy of each laser ray across the interfacial grid cells it traverses. A convergence study presented in Appendix F further demonstrates that the selected ray discretization is sufficient to ensure that the predicted melt track morphology and temperature profiles exhibit consistent convergence behavior.

In the present study, a standard Gaussian beam profile is adopted to represent the spatial distribution of the incident laser energy. The influence of alternative beam spatial distributions is beyond the scope of the present study [78] and will be investigated in future studies. It should be noted that the ray-tracing framework is formulated in a general manner, with the laser energy distribution introduced as an input parameter. Alternative heat source profiles (e.g., top-hat or super-Gaussian beams) can be readily incorporated into the present framework to investigate the influence of laser characteristics on melt pool behavior [79,80]. Such parametric studies, however, are beyond

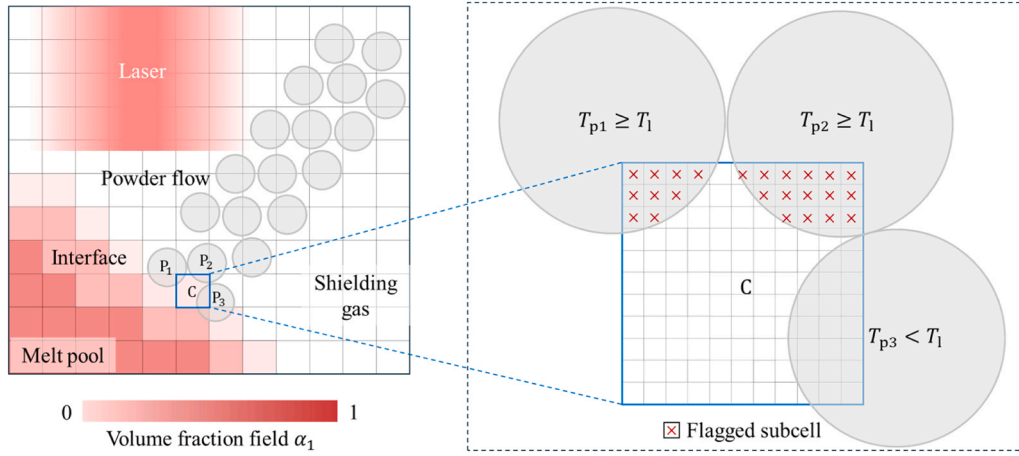


Fig. 4. Schematic of the proposed multiphase model for PB-DED. The right panel shows a magnified view of Cell C and particles P_1 , P_2 , and P_3 from the left panel, illustrating the subcell decomposition of Cell C and the labeling strategy: a particle is converted into CFD fluid only when its temperature exceeds the liquidus temperature and it has detached from the melt pool interface, after which the sub-grids overlapping with the particle within the interface cell are flagged.

the scope of the current work, which focuses primarily on demonstrating the feasibility and accuracy of the proposed computational framework.

A central challenge in this semi-resolved framework is the unified treatment of laser interaction with two fundamentally different interface types: the sharply defined surfaces of DEM particles and the diffuse interface of the VOF-captured fluid. This necessitates a hybrid ray-tracing strategy to consistently model Fresnel reflection and refraction. The distinction arises from the inherent characteristics of each phase: (1) DEM Particles are geometrically defined with sharp interfaces (known center and radius), allowing for analytical calculation of reflection points and the direct assignment of all refracted energy to the particle's single temperature; (2) The Fluid Interface is a diffuse region where the metal volume fraction transitions from 0 to 1. This requires a specialized approach to determine the effective reflection point and to distribute the refracted laser energy across multiple interfacial cells based on local volume fraction and absorption laws. Our model explicitly bridges this gap, enabling physically consistent laser energy deposition across both dispersed and continuum phases within a single, unified simulation. The computational steps of the laser ray tracing model in PB-DED are provided in [Appendix C](#).

The ray-tracing model operates on the diffuse melt pool surface reconstructed from the VOF interface. The dynamic topology of the melt pool surface is therefore naturally captured by the evolution of the VOF interface, enabling the ray-tracing algorithm to account for multiple reflections and local variations in surface orientation. In the present implementation, the effective absorption coefficient ε is evaluated using a Fresnel-based approximation for metallic surfaces; the detailed formulation and verification of this absorption model have been extensively discussed in our previous work [77]. For the material systems considered in this study, the thermophysical properties and optical parameters for Ti-6Al-4V and AISI 304 stainless steel follow the values reported in Refs. [32,81,82] and [83].

Since the procedures described above involve ray-grid and ray-particle intersection detection, we briefly describe how these operations are efficiently implemented on the GPU using a spatial hashing algorithm and the Digital Differential Analyzer (DDA) method. First, the entire computational domain is discretized into uniform grid cells via a spatial hashing algorithm. Second, all particles and fluid cells are assigned to their corresponding hash grid cells based on spatial coordinates. Finally, the DDA algorithm is employed to efficiently traverse the hash grid cells along the ray path. During traversal, each hash cell is checked for the presence of particles or fluid interface cells that meet the interaction criteria. If present, the corresponding intersection calculations are performed.

2.2. Multiphase modeling of melt pool dynamics with particle-fluid phase transition

2.2.1. Multiphase model

PB-DED is a sophisticated additive manufacturing process that employs a laser beam to melt powder particles delivered via a shielding gas onto a solid substrate, resulting in the formation of a molten pool which subsequently solidifies into a deposited track. This highly dynamic process is governed by multiphase flow, involving the solid substrate, powder particles, molten metal, and ambient gas, alongside multiple phase transformations, namely melting, solidification, and vaporization. In the present study, the powder carrier gas and the shielding gas are assumed to be identical and are therefore treated as a single gaseous phase, leading to a two-phase formulation.

We herein employ the volume of fluid (VOF) method in conjunction with the sharp interface capture scheme, MULES, coupled further with DEM to furnish such an integrated computational framework for modeling of such a multiphase system involving in DED. As a default scheme in *OpenFOAM* [84], MULES treats the smeared interface (Fig. 4) by adding a compressive flux term $\nabla \cdot (\alpha_i(1 - \alpha_i)\mathbf{u}_c)$ into the LHS of the advection equation of phase i [85]. The MULES scheme is adopted here due to its numerical robustness and computational efficiency, which makes it suitable for large-scale multiphase simulations within the present GPU-parallel framework.

$$\frac{\partial \varepsilon \alpha_i}{\partial t} + \nabla \cdot (\varepsilon \alpha_i \mathbf{u}) + \nabla \cdot (\alpha_i(1 - \alpha_i)\mathbf{u}_c) = 0, \quad (26)$$

where the subscript i denotes fluid phase 1 or 2 (e.g., melt liquid and ambient gas). $\mathbf{u}_c = (c_M \varepsilon |\nabla \alpha_i| / |\nabla \alpha_i|)$ is the compressed velocity, α_i is the volume fraction of phase i , and $c_M \in (0, 1)$ is the coefficient to control the compressed velocity. In the present implementation, the convective flux term $\nabla \cdot (\varepsilon \alpha_i \mathbf{u})$ is discretized using the Van Leer scheme to ensure boundedness and improved interface resolution. For the compressive flux term $\nabla \cdot (\alpha_i(1 - \alpha_i)\mathbf{u}_c)$, a split discretization strategy is adopted: the term $\nabla \cdot (\alpha_i \mathbf{u}_c)$ is discretized using an upwind scheme, while $\nabla \cdot ((1 - \alpha_i)\mathbf{u}_c)$ is discretized using a downwind scheme to enhance interface sharpening while maintaining numerical stability.

The equivalent density ρ and viscosity μ in the momentum equation and the thermal conductivity k and heat capacity C in the Temperature equation over the entire domain could be written as:

$$\begin{cases} \rho = \alpha_1 \rho_1 + \alpha_2 \rho_2 \\ \mu = \rho(\alpha_1 \mu_1 / \rho_1 + \alpha_2 \mu_2 / \rho_2) \\ k = \alpha_1 k_1 + \alpha_2 k_2 \\ C = (\alpha_1 \rho_1 C_1 + \alpha_2 \rho_2 C_2) / \rho \end{cases}, \quad (27)$$

Accurate calculation of the contact angle at solid boundaries is crucial in two-phase flow simulations, as it directly influences the precision of interface capturing and related physical processes. Within the VOF framework, the prescribed contact angle is enforced by reconstructing the interface normal vector, denoted as $\mathbf{n}_c$, on boundary faces. The curvature is then obtained as the negative divergence of this normal vector, which is subsequently used to compute the surface tension force, as shown in Eq. (1). This term is derived from enforcing two constraints: orthogonality and angular continuity. Specifically, the reconstructed interface normal vector $\mathbf{n}_c$ must satisfy $\mathbf{n}_c \cdot \mathbf{n}_{\text{wall}} = \cos \theta_{\text{eq}}$ and $\mathbf{n}_c \cdot \mathbf{n} = \cos \Delta\theta$. $\Delta\theta$ is the angle difference between the target contact angle θ_{eq} and the current contact angle θ_{now} . θ_{now} is defined as $\theta_{\text{now}} = \arccos(\mathbf{n} \cdot \mathbf{n}_{\text{wall}})$. By solving this system of equations, this adjusted normal vector $\mathbf{n}_c$ is defined as a linear combination:

$$\begin{cases} \mathbf{n}_c = a\mathbf{n}_{\text{wall}} + b\mathbf{n} \\ a = \frac{\cos\theta - \cos\theta_{\text{now}} \cdot \cos\theta}{1 - (\cos\theta_{\text{now}})^2} \\ b = \frac{\cos\Delta\theta - \cos\theta_{\text{now}} \cdot \cos\theta}{1 - (\cos\theta_{\text{now}})^2} \end{cases}, \quad (28)$$

where $\mathbf{n}_{\text{wall}}$ denotes the unit normal vector of the solid boundary.

2.2.2. Thermal-induced phase changes

In PB-DED, the dominant phase-change modes are melting and solidification, which occur primarily through conduction. This contrasts with LPBF, where intense vaporization often leads to keyhole-mode melting. Therefore, while recoil pressure and evaporative heat loss are included, the vapor phase is not explicitly resolved, consistent with prior modeling approaches [77]. The solid phase is treated as a highly viscous fluid, with the viscosity varying smoothly between solid and liquid states via a temperature-dependent function:

$$\ln\mu = \frac{1}{2} \operatorname{erfc} \left[\frac{4}{\ln T_1 - \ln T_s} \cdot \left(\ln T - \frac{\ln(T_1) + \ln(T_s)}{2} \right) \right] \cdot (\ln\mu_s - \ln\mu_l) + \ln\mu_l, \quad (29)$$

where μ_s and μ_l denote the viscosities corresponding to the solidus T_s and liquidus T_l temperatures, respectively, and $\operatorname{erfc}(\cdot)$ represents the complementary error function.

During PB-DED, powder particles travel from the nozzle to the laser focal zone and undergo rapid heating. Depending on laser power, powder feed rate, and particle-size distribution, particles may arrive at the melt pool in solid, partially molten, or fully molten states [46,86]. In this work, we adopt a simplified modeling strategy: all in-flight particles remain within the Lagrangian DEM framework regardless of their phase state. Transition to the Eulerian CFD fluid phase occurs only when a particle impacts the melt track and its local temperature exceeds the liquidus temperature. This “delayed-transition” approach is justified by the following physical and numerical considerations:

- (1) **Dominance of Surface Tension (Particle Shape):** Experimental observations confirm that in-flight molten droplets maintain a spherical or near-spherical morphology due to the dominance of surface tension at the microscale [87]. This can be rigorously quantified using dimensionless scaling analysis. For a representative Ti-6Al-4V droplet (diameter $d_p = 50 \mu\text{m}$, density $\rho_p = 4,420 \text{ kg/m}^3$, surface tension $\sigma = 1.5 \text{ N/m}$, with $d\sigma/dT = -2.6 \times 10^{-4} \text{ N/(m}\cdot\text{K)}$), the gravitational influence is negligible, as indicated by the exceedingly small Bond number $\text{Bo} = \rho g R^2 / \sigma \approx O(10^{-4})$. Furthermore, the aerodynamic forces generally remain insufficient to induce significant deformation, as the Weber number ($\text{We} = \rho u^2 d_p / \sigma$) typically remains well below the critical breakup threshold ($\text{We}_c \approx 12$) [88] in standard DED

carrier gas flows. Consequently, the Laplace pressure ($\Delta P = 2\sigma/R$) generates a restoring force that vastly overwhelms inertial and Marangoni effects ($F_M \approx (d\sigma/dT)\Delta T d_p$, estimated to be two orders of magnitude smaller), thermodynamically favoring a spherical equilibrium shape. Thus, representing molten droplets as spherical DEM elements is a physically consistent approximation.

- (2) **Collision Dynamics and Coalescence:** Unlike the instantaneous elastic-frictional contact between solid particles, interactions involving molten droplets are governed by viscous dissipation and surface tension-driven coalescence. In flight, molten droplets tend to merge upon impact rather than rebound [87,89]. To emulate this inelastic behavior within the DEM framework, particles reaching the liquidus temperature are assigned a near-zero coefficient of restitution [90]. This effectively suppresses post-collision rebound, approximating the kinetic energy dissipation characteristic of viscous fluids. While this approach simplifies the complex topological changes of droplet merging (e.g., oscillation damping), it correctly captures the aggregate mass and enthalpy flux delivery to the melt pool. Since the individual particle diameters are typically less than 4% of the melt-track width, macroscopic track morphology is governed by global mass/energy conservation rather than the micro-morphology of individual incident droplets. Crucially, this simplification avoids the prohibitive computational cost associated with fully resolving droplet spreading dynamics, which would increase the simulation workload by more than two orders of magnitude ($>100\times$). The feasibility and accuracy of this efficient approach are subsequently validated in Section 3.4, where close agreement between our simulated track geometries and experimental measurements confirms that the assumption yields physically realistic results without introducing significant artificial mass accumulation.
- (3) **Grid Resolution and Numerical Fidelity:** The decision to retain molten particles within the Lagrangian framework is primarily dictated by the spatial discretization constraints inherent to the semi-resolved CFD-DEM coupling scheme. In this regime, the fluid grid size (Δx) is comparable to the particle diameter ($d_p \approx \Delta x$). Standard VOF method and resolved CFD-DEM method require a fine mesh (typically $d_p/\Delta x > 8 \sim 10$) to accurately resolve interface curvature and suppress parasitic currents [56, 91]. Converting an in-flight droplet into the Eulerian fluid phase at the current coarse resolution ($d_p/\Delta x \approx 1$) would induce severe numerical diffusion. This would result in an artificially diffuse interface smearing across multiple control volumes, fundamentally compromising the geometric fidelity of the droplets. By postponing the Eulerian conversion until the particle impinges upon the melt pool, this study leverages the following advantages:
 - (i) **Computational efficiency:** The approach reduces the computational burden by approximately two orders of magnitude compared to fully resolved CFD-DEM approaches [56], while preserving the macroscopic accuracy of mass and momentum transfer.
 - (ii) **Ray-tracing precision:** The DEM representation maintains a sharp, explicit geometric boundary defined by the particle radius. This “sharp-interface” description is numerically imperative for the ray-tracing algorithm, which relies on well-defined surface normal vectors to compute Fresnel absorption and multi-scattering effects. In contrast, the diffuse interface generated by a coarse-grid VOF reconstruction would obscure the exact surface topology, leading to significant errors in laser energy coupling calculations.

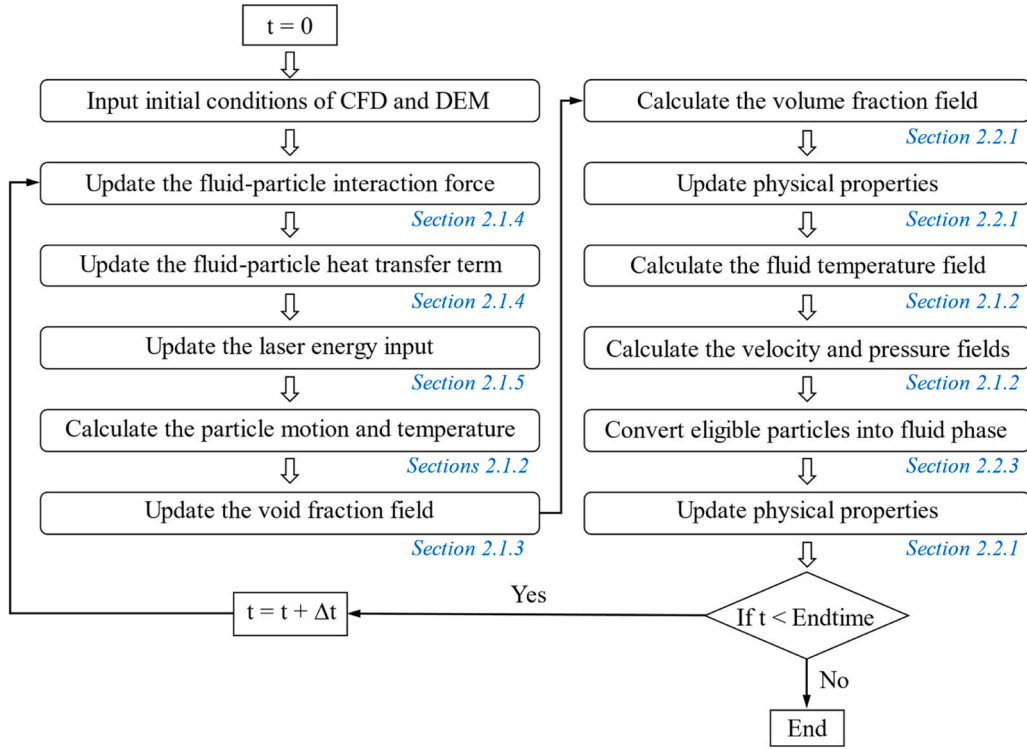


Fig. 5. Flowchart of the proposed multiphase semi-resolved CFD-DEM framework for PB-DED, with blue text indicating corresponding sections.

2.2.3. Conservation during particle-to-fluid phase transition

When a particle reaches the liquidus temperature and enters the melt track, it is transferred to the continuum fluid phase. To ensure physical consistency, the conversion enforces local conservation of mass, momentum, and energy, updating the fluid volume fraction, velocity, and temperature in the affected control volumes. Because the particle diameter is comparable to the CFD cell size, a single particle may span multiple cells. A spatial-subdivision method, designed for efficient

GPU-parallel computation, is adopted to accurately distribute the particle's contribution. The conservation procedure is given in Appendix B.

2.3. Overall solution procedure

The computational framework for the multi-phase semi-resolved CFD-DEM for high-fidelity modeling of powder-based directed energy deposition is illustrated in Fig. 5. The momentum equation of CFD is

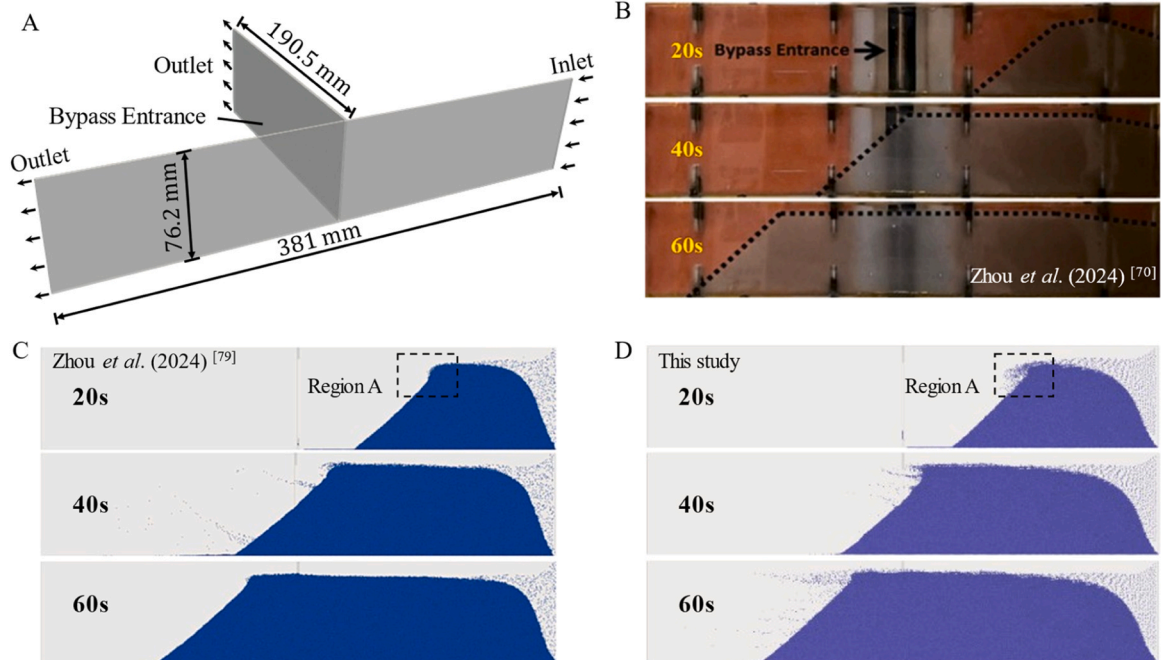


Fig. 6. (A) Schematic illustration of the proppant transport model. Comparison between (B) experimental observations [93], (C) the simulation results obtained using the CFDEM software (unresolved CFD-DEM) [93], and (D) the predictions of the present work (semi-resolved CFD-DEM) at 20 s, 40 s, and 60 s.

solved using the Pressure Implicit with Splitting of Operators (PISO) algorithm to ensure accurate velocity-pressure coupling [92]. The proposed algorithm has been fully integrated into TFluid (www.t-fluid.com), a full-process GPU-accelerated CFD-DEM simulation platform. All computational modules described in Sections 2.1 and 2.2 have been parallelized on the GPU. The assembly of governing equations and intermediate computational procedures are implemented using CUDA C++. The sparse linear systems arising from the discretized equations are solved using the NVIDIA AmgX library (version 2.4.0), and the simulation results are exported using the VTK library (version 9.1) for visualization and post-processing. The corresponding computational efficiency will be demonstrated in the illustrative case presented later. In the present simulations, the residual thresholds for both the momentum and energy equations were set to 1×10^{-13} , and sufficient inner iterations were performed at each time step to ensure that the prescribed convergence criterion was satisfied. Further details on the discretization strategies and GPU-parallel numerical algorithms can be found in our previous work [54], where the computational framework is described in greater depth. The workflow is described in detail in Appendix D.

It should be noted that the current implementation of the TFluid framework does not yet support multi-GPU parallelization. As a result, the maximum problem size is limited by the memory capacity of a single GPU. For instance, a computational domain with approximately 1 million cells requires around 2 GB of GPU memory. Developing an efficient multi-GPU strategy is a subject of ongoing research, and it remains to be determined whether traditional domain-decomposition approaches would be optimal for extending the scalability of the framework. This limitation is important for users intending to simulate very large domains or highly resolved melt pool dynamics. To further facilitate large-scale simulations, we have previously developed a fully GPU-based AMR algorithm [55] to selectively refine key regions, such as the melt pool, while maintaining computational efficiency.

3. Benchmark and validation

This section presents a systematic validation of the proposed computational framework through four benchmark cases. Each case targets a specific physical module: (1) proppant transport to assess the semi-resolved CFD-DEM coupling; (2) bare plate laser melting to validate the ray-tracing and melt pool dynamics; (3) contact angle analysis to verify interfacial wetting behavior; and (4) full PB-DED to test the integrated thermal dynamics and final track morphology. Collectively, these benchmarks demonstrate the framework's comprehensive capability in capturing the coupled multi-physics of PB-DED, from powder-stream interaction to energy deposition and solidification.

3.1. Validation of semi-resolved CFD-DEM approach

To validate the semi-resolved CFD-DEM approach, we first examine the interaction between the fluid and proppant particles during transport. Fig. 6 A illustrates a simplified T-shaped fracture model with one inlet and two outlets, where one outlet serves as a bypass entrance. Both the fluid and the proppant particles are injected through the inlet. The main fracture length is 381 mm, while the secondary fracture length is 190.5 mm. The fracture height and width are 76.2 mm and 2 mm, respectively. The proppant particles have a density of 2650 kg/m^3 and a diameter of 0.6 mm, with a mass injection rate of 0.9516 g/s. The carrier fluid has a density of 998.2 kg/m^3 and a viscosity of $0.001 \text{ Pa}\cdot\text{s}$, and it is injected at a velocity of 0.1 m/s.

The CFD computational domain was discretized using hexahedral grids with a uniform cell size of 1 mm, corresponding to approximately 1.67 times the particle diameter, resulting in a total of 87,248 cells. The CFD time step was set to $2.5 \times 10^{-4} \text{ s}$, while the DEM time step was $2.5 \times 10^{-5} \text{ s}$. For the DEM particles, the Young's modulus was $5.0 \times 10^6 \text{ Pa}$, with a friction coefficient of 0.5 and a restitution coefficient of 0.7. The

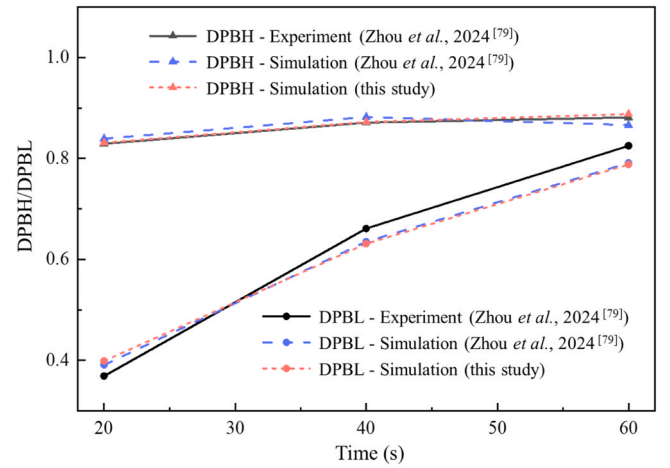


Fig. 7. Comparison of Dimensionless Proppant Bank Height (DPBH) and Dimensionless Proppant Bank Length (DPBL) between experimental measurements [93], existing numerical results [93], and the current simulations.

DEM particles were uniformly injected from the right-hand inlet, as shown in Fig. 6D.

Fig. 6B-D present the particle distribution in the main fracture at three time instants, comparing the experimental observations [93], existing simulation results [93], and the present semi-resolved CFD-DEM results. As time progresses, the continuously injected particles transported by the fluid accumulate within the computational domain, leading to the formation of proppant banks. Fig. 7 provides a quantitative comparison of two key metrics: the Dimensionless Proppant Bank Height (DPBH) and the Dimensionless Proppant Bank Length (DPBL). The DPBH is defined as the ratio of the proppant bank height to the fracture height, while the DPBL is defined as the ratio of the proppant bank length to the main fracture length. For DPBH, the maximum deviations of the present simulation from the experimental data and the existing simulation results across three time instants are 0.8% and 2.5%, respectively. For DPBL, the corresponding deviations are 4.5% and 2.0%. All deviations remain within acceptable bounds, thereby validating the accuracy of the present simulation results.

Furthermore, by comparing Fig. 6 C and D, notable differences can be observed at the apex of the particle pile (Region A in Fig. 6 C and D). To investigate this, we analyzed the phenomena of particle splashing and local accumulation in this region, as illustrated in Fig. 8. The results indicate two primary contributing factors: (1) the presence of the particle pile restricts fluid outflow to a narrow region at the top, particularly at the apex of Region A, where high-velocity fluid further entrains particles, causing them to splash forward; (2) as the fluid exits through this narrow region, it interacts with the sloped front of the particle pile, forming a triangular zone where a pronounced vortex develops. This vortex impedes the forward motion and downward settling of particles driven by gravity, leading to local particle accumulation in Region A. Consequently, all three time frames in Fig. 6D show clear particle buildup in this region. Although similar phenomena have been reported in previous simulations, they were less pronounced than in the present study. We attribute this difference to our use of a semi-resolved CFD-DEM approach with a finer grid spacing of 1 mm, compared with the 3 mm coarse grid used in unresolved CFD-DEM studies. This finer resolution is particularly critical for capturing the fluid dynamics in the narrow top region of the particle pile, which has an average height of only 9 mm.

3.2. Validation of contact angle model

The wetting behavior between the molten metal and the substrate critically influences the stability and morphology of the deposited melt

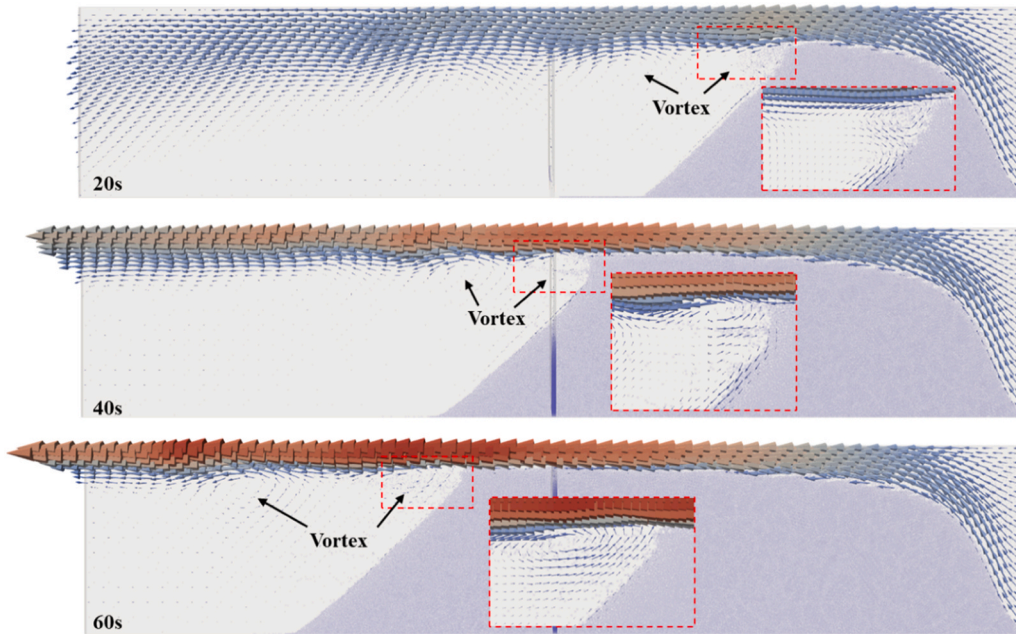


Fig. 8. Semi-resolved CFD-DEM predictions of the fluid velocity vector fields at 20 s, 40 s, and 60 s.

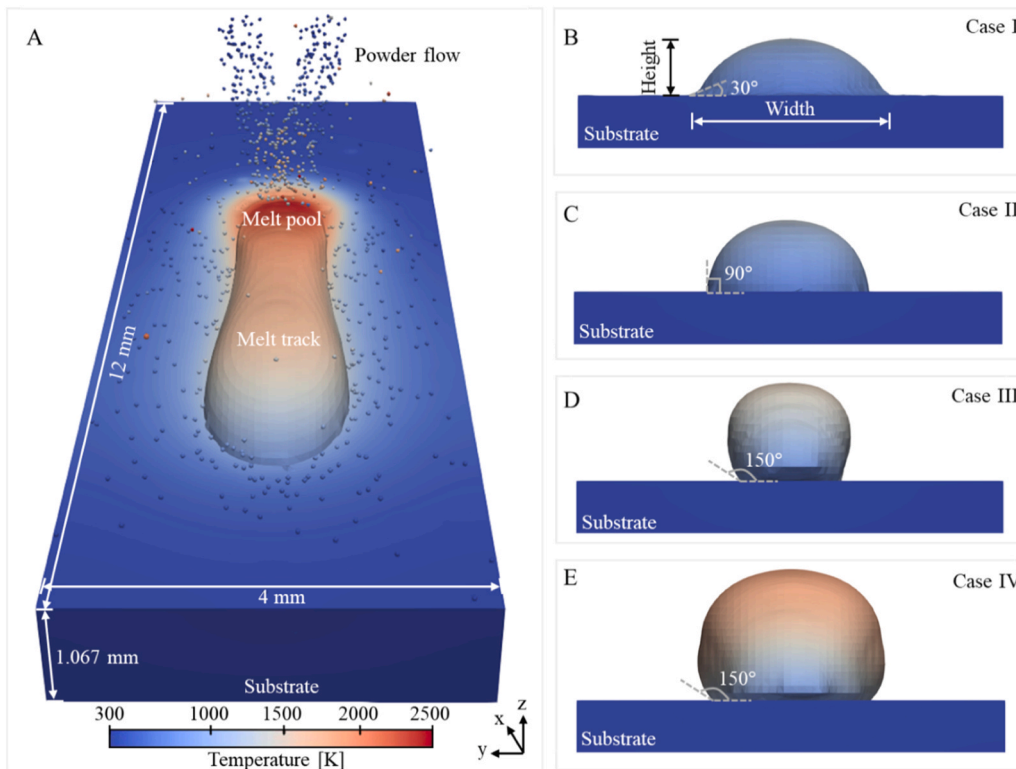


Fig. 9. Simulation results of the contact angle test: (A) schematic of the model (dimensions in mm); (B) side views of Cases I-IV, showing clear differences in contact angles (β).

track during the DED process. This behavior is commonly characterized by the contact angle at the solid-liquid-gas triple junction, which reflects the balance of interfacial energies among the three phases. Variations in the contact angle can significantly affect melt spreading, track continuity, and the propensity for balling phenomena. Moreover, the contact angle is influenced by practical factors such as substrate material [94], surface oxidation condition [95], and substrate temperature [96]. Therefore, investigating the influence of the contact angle is important

for understanding melt track formation mechanisms and assessing the capability of the proposed numerical framework to capture wetting-related phenomena.

In this DED numerical example, Ti-6Al-4V powder was employed, with material properties detailed in [Tables E.1 and E.2](#) of the [Supplementary Materials](#). To isolate and validate the proposed contact model, mono-sized particles with a diameter of 50 μm were adopted. The particles were injected with an initial velocity vector of (0, -1, -5)

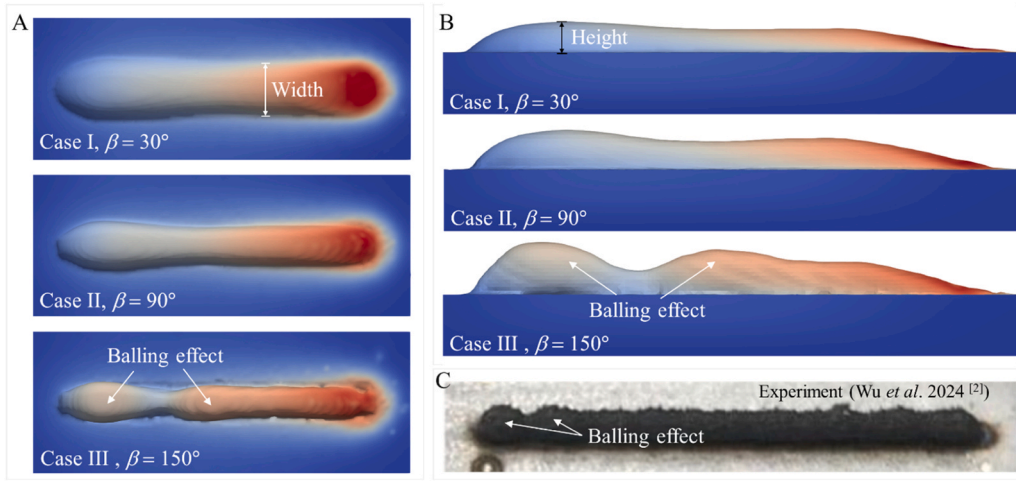


Fig. 10. Comparison of simulated melt geometries with contact angle β equal to 30° , 90° and 150° (Cases I-III): (A) top view in the x-y plane and (B) front view in the x-z plane. (C) Experimentally observed melt track [2]. The color contour is consistent with that in Fig. 9.

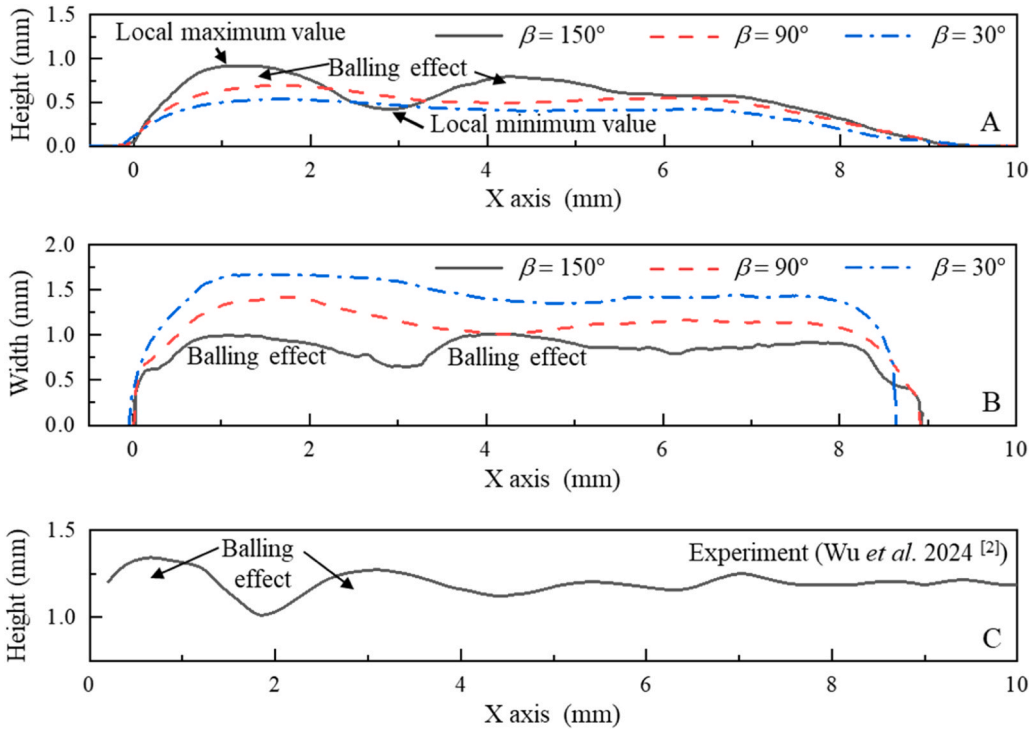


Fig. 11. (A) Variation of the melt track height (Z axis) along the $y = 0$ cross-section; (B) variation of the melt track width (Y axis) along the $z = 0.15$ mm cross-section; (C) experimentally measured variation of the melt track height along the track length direction [2].

m/s, as illustrated in Fig. 9 A. A discrete injection strategy was implemented where eight particles were released from each side every $20 \mu\text{s}$, yielding a total mass flow rate of approximately 1.7×10^{-5} kg/s. The laser power was maintained at 1000 W with a beam radius of $750 \mu\text{m}$. Both the powder stream and the laser source traversed along the positive x-direction at a scanning speed of 0.3 m/s. As the particles melted and coalesced continuously, a melt track gradually formed on the substrate.

To assess the model's fidelity in capturing the contact angle (β), four distinct simulation scenarios were established. Cases I-III examined the effect of wettability by varying the contact angle to 30° , 90° , and 150° , respectively. In Case IV, the mass flow rate was doubled (injection interval reduced to $10 \mu\text{s}$) to investigate the interplay between deposition volume and contact morphology. Fig. 9B-E display the side views of the melt tracks at 86 ms. The results demonstrate that the proposed model

accurately reproduces the prescribed contact angles on the substrate. Notably, under the lower mass flow rate (Case III, Fig. 9D), the melt track with a high contact angle (150°) exhibits a less cohesive morphology compared to the higher mass flow case (Case IV, Fig. 9E). This discrepancy arises because, at a lower feed rate, the insufficient molten volume undergoes rapid cooling at the substrate interface. This thermal condition restricts spreading and coalescence, leading to a thinner, discontinuous track. Conversely, increasing the mass flow rate provides sufficient thermal mass to sustain the molten state longer, resulting in a fuller and more distinct high-contact-angle morphology.

Fig. 10 A and B present orthogonal views (front and top) of Cases I-III. It is evident that low contact angles favor the formation of flat, continuous tracks, whereas high contact angles (e.g., 150°) induce a pronounced balling effect. As the contact angle increases, the melt track

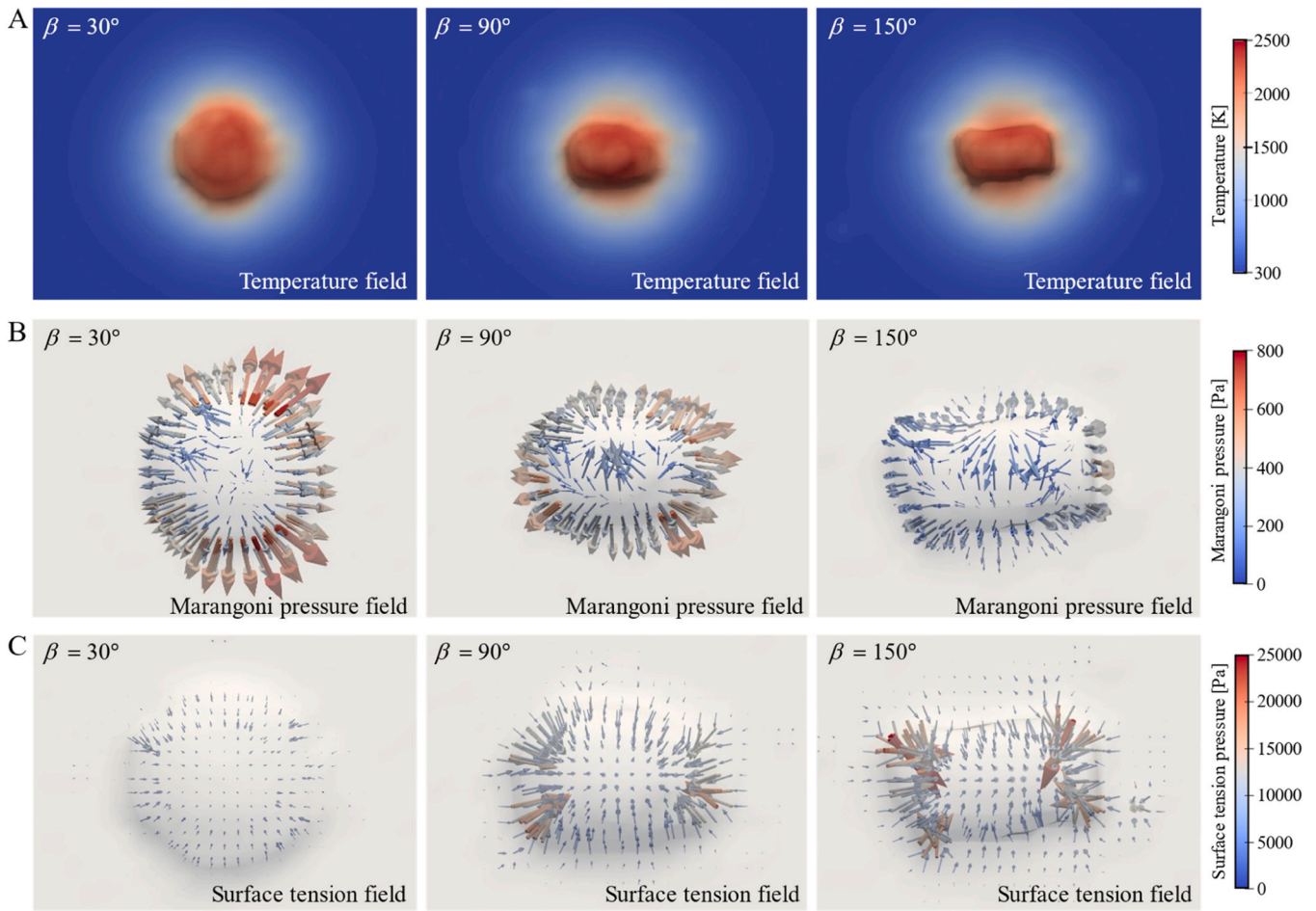


Fig. 12. Simulated results at $t = 3$ ms for three contact angles (30° , 90° , and 150°): (A) melt-track morphology and temperature field, (B) Marangoni-driven pressure field, and (C) surface tension-driven pressure field.

cross-section transitions towards a circular geometry. This is accompanied by an increase in cross-sectional height, a reduction in width, and intensified height fluctuations along the scanning direction. These simulation results correlate well with the experimental observations by Ref. [2], which stated that increased contact angle promotes balling defects. A representative experimental instance of this phenomenon is shown in Fig. 10 C, which bears a strong morphological resemblance to the simulated result for the high contact angle case.

Quantitative assessment further corroborates these morphological trends. Fig. 11 A and B plot the variations in melt track height (z -coordinate along $y = 0$ cross-section) and width (y -coordinate along $z = 0.15$ mm cross-section), respectively. The peak-to-valley height difference, defined as Δh (see Fig. 11), serves as a metric for track uniformity. For contact angles of 30° , 90° , and 150° , the computed Δh values are 0.133 mm, 0.200 mm, and 0.493 mm, respectively. The substantial increase in Δh at higher contact angles quantifies the severity of the balling instability. This trend aligns with experimental data [2], where a comparable Δh of 0.332 mm was recorded (Fig. 11 C). Concomitantly, the intensified balling behavior at high contact angles significantly constrains the track width. As detailed in Fig. 11B, the average widths within the stable region ($x \in [1, 8]$ mm) are 1.49 mm, 1.17 mm, and 0.87 mm for the three respective cases. Notably, the track width at $\beta = 150^\circ$ is approximately 58% of that at $\beta = 30^\circ$, highlighting the significant narrowing effect induced by increased wettability resistance.

A comparative analysis was conducted to elucidate how the melt-track morphology varies under the three prescribed contact angles. The evolution of the melt pool was examined with focus on the two

dominant driving forces: Marangoni pressure and surface tension (Fig. 12 and Fig. 13). At the early deposition stage ($t = 3$ ms, Fig. 13), Marangoni pressure decreases with increasing contact angle, whereas surface tension increases, yielding up to a fourfold difference. As schematized in Fig. 12B-C, Marangoni's pressure promotes lateral spreading, while surface tension drives inward contraction. In magnitude, the equivalent pressure from surface tension nearly surpasses that from the Marangoni's effect by a factor of twenty. Consequently, melt-track morphology is predominantly governed by surface-tension-driven flow, despite a non-negligible Marangoni contribution.

This mechanism becomes more pronounced at high contact angles. As illustrated in Fig. 12 C, the interface between the melt track and the substrate experiences an exceptionally large surface-tension-induced pressure, up to 25,000 Pa. This inward-directed force draws the molten material from the boundary toward the track center, thereby reducing the overall melt-track width, consistent with the morphology observed in Fig. 11. These results collectively demonstrate that surface tension plays a decisive role in shaping the melt-track profile, particularly under conditions of high contact angle.

The surface-tension distribution and velocity field along the longitudinal cross-section (A-A in Fig. 13 A) at 30 ms are shown in Fig. 13C-D. While surface tension acts normal to the melt-gas interface in all cases, its magnitude at the leading edge (the active laser-irradiation zone) is markedly intensified under high contact angles (90° and 150°), reaching values two to three times higher than in surrounding areas due to a transient deviation from the equilibrium contact angle. The resultant flow field (Fig. 13D) reveals that this elevated surface tension drives molten metal laterally toward the left-side lobe. This

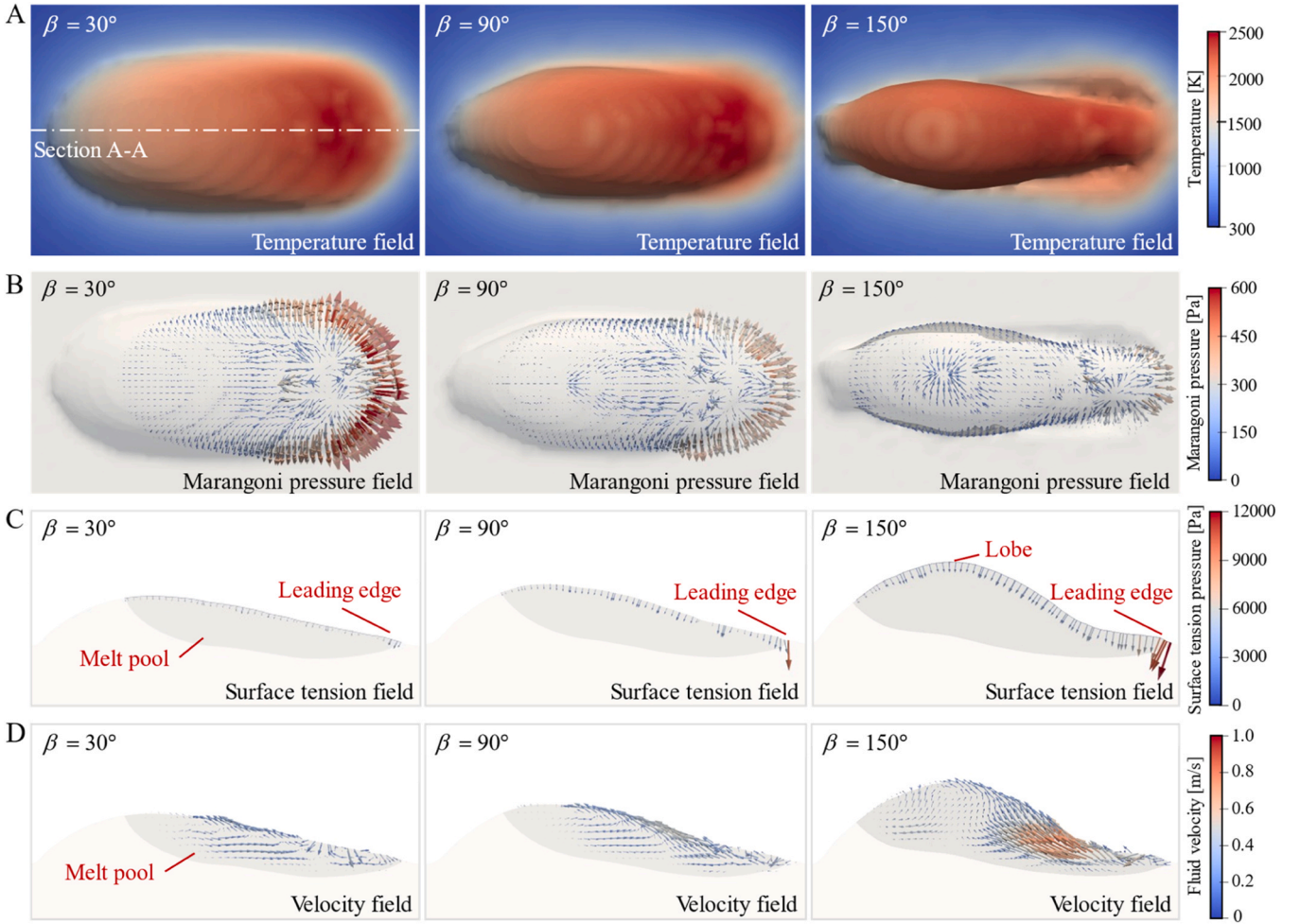


Fig. 13. Simulated results at $t = 30$ ms for three contact angles (30° , 90° , and 150°): (A) melt-track morphology and temperature field, (B) Marangoni-driven pressure field, (C) surface-tension field along section A-A (with vector arrows), and (D) velocity field along section A-A (with vector arrows).

forcing intensifies with contact angle, producing a peak flow velocity in the 150° case approximately double that of the 30° case and leading to a significantly enlarged lobe.

To further investigate the origin of balling, melt-pool flow dynamics were analyzed for contact angles of 90° and 150° via temporal snapshots (Fig. 14 and Fig. 15). For 90° (Fig. 14), the flow structure remains consistent: surface-tension imbalance at the leading edge drives metal into the left-side lobe, forming a vortex at the transition region. This persistent, repeating process results in a continuous, uniform track (Fig. 10). In contrast, the 150° case (Fig. 15) exhibits dynamic instability. The intensified leading-edge surface tension generates a stronger lateral push, leading to higher flow velocities. The resulting vortex zone becomes compressed and shifts toward the lobe's mid/rear section. The enlarged lobe accumulates material until a neck forms (e.g., at 40 and 50 ms), effectively bifurcating the melt pool. Surface tension then fosters two opposing vortices on either side of the neck, blocking melt transfer from the leading edge to the initial lobe and promoting a new lobe downstream. This new lobe eventually mirrors the flow behavior of the first, completing a cycle of lobe formation and separation.

In summary, high contact angles induce strong surface tension at the leading edge, which significantly alters the internal flow structure of the melt pool. The resulting vortex localization near the lobe center enhances lobe growth, ultimately causing the formation of a neck and subsequent separation into two lobes, a fundamental mechanism underpinning the balling effect. This conclusion is in agreement with existing experimental observations [2], which report that an increased contact angle of the molten material displaces new deposition away

from the leading edge of previously deposited liquid, leading to discontinuous bead formation and promoting the balling defect in linear deposits. The present simulation not only corroborates this mechanism but also provides a quantitative and dynamic description that is difficult to obtain experimentally, such as detailed alterations in the internal melt pool flow, localized vortex evolution, and their direct role in lobe growth and separation, thereby offering a more comprehensive and mechanistic insight into the balling phenomenon.

3.3. Validation of ray-tracing model

The ray-tracing model is pivotal for accurately predicting the spatiotemporal distribution of laser energy absorption by both the feedstock particles and the evolving melt pool. The absorbed energy directly dictates the local thermal field, driving the thermodynamic behavior of the melt pool, including phase transitions and Marangoni-driven convection. Consequently, the fidelity of the ray-tracing algorithm is decisive in determining the thermal history and the resulting solidified morphology. Even minor inaccuracies in the optical energy coupling can lead to significant deviations in the predicted melt pool dimensions and surface topology.

To ensure the reliability of the proposed framework, this section presents a quantitative validation of the ray-tracing implementation against experimental benchmarks. Specifically, the predicted temperature distributions and melt pool geometries are rigorously evaluated against corresponding experimental measurements. This validation is essential to confirm that the model correctly captures the complex

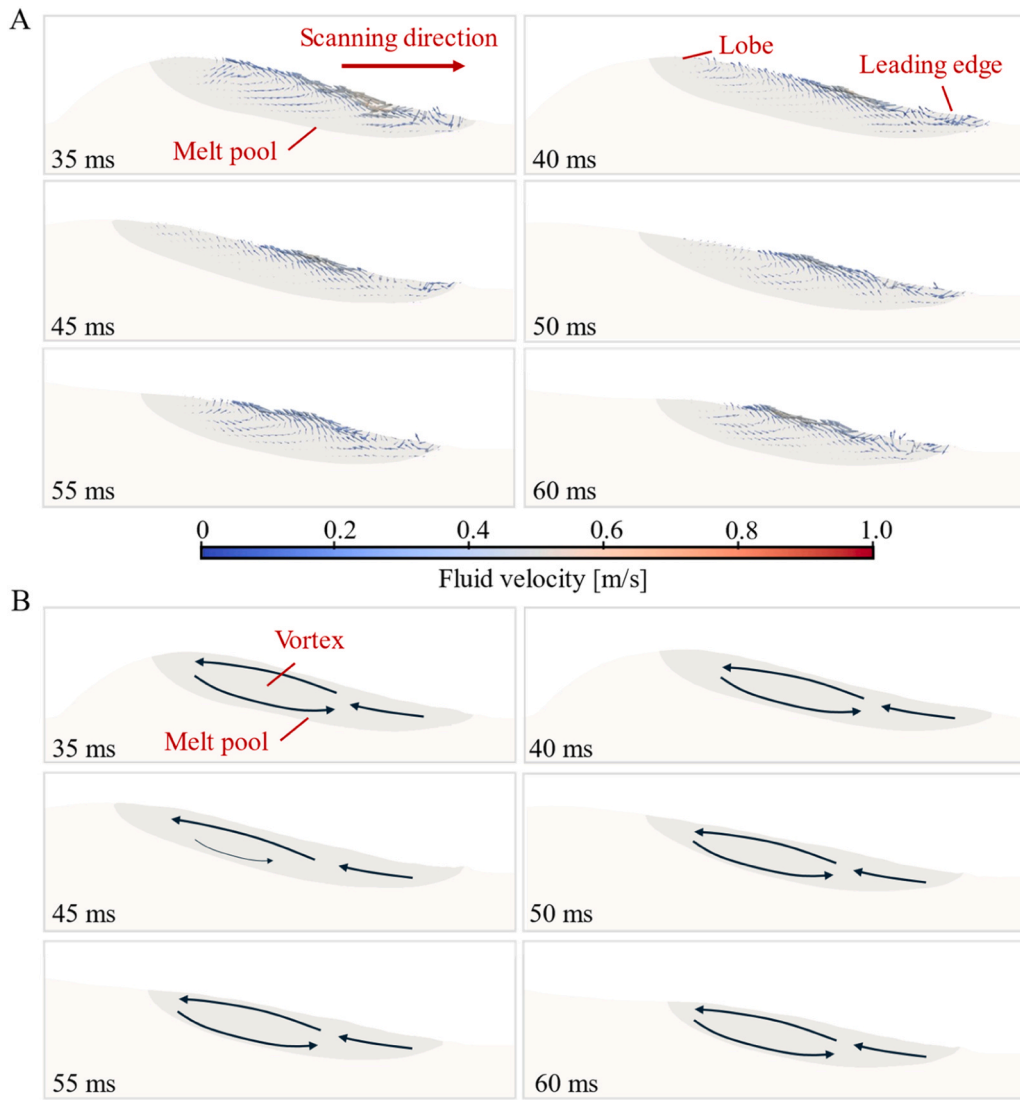


Fig. 14. Simulated results for a contact angle of 90° at six time instants: (A) velocity field along section A-A, and (B) schematic of melt-pool flow patterns along section A-A. Note: the position of section A-A is illustrated in Fig. 13 A.

energy transfer mechanisms governing the interactions between the incident laser, the in-flight metallic particles, and the dynamic melt pool. Two distinct validation cases are examined: bare plate heating and powder stream heating.

3.3.1. Bare plate heating

The first benchmark involves the laser melting of a bare Ti–6Al–4V substrate under constant scanning speeds, a standard configuration for investigating melt pool evolution without the complexity of powder addition. The thermophysical and optical properties of Ti–6Al–4V are detailed in Tables E.1 and E.2, respectively. The processing parameters, covering a range of laser powers and scanning speeds for the eight validation cases, are summarized in Table E.3. The computational domain was defined with a fixed width of $300\ \mu\text{m}$ and a uniform grid size of $3.75\ \mu\text{m}$, while the domain length and height were adjusted dynamically to accommodate the varying scanning speeds and melt pool depths. A detailed mesh sensitivity analysis for the present numerical framework can be found in our previous study [32], where the influence of grid resolution on the predicted melt pool characteristics was systematically evaluated. An adaptive time-stepping scheme was employed, governed by the Courant-Friedrichs-Lewy (CFL) condition, with the Courant number strictly capped at 0.5 to ensure numerical

stability.

It should be noted that, although similar benchmark configurations were investigated in our previous work [77], the numerical framework adopted in the present study differs significantly. The current solver is a fully GPU-resident implementation developed in CUDA C++, with the governing equations, VOF interface capturing scheme, and laser ray-tracing model all redesigned to exploit massive parallelism on GPUs. Additionally, the present study employs the MULES algorithm for interface capturing, and vaporization effects are not explicitly considered. A dedicated validation of melt pool morphology is therefore necessary to demonstrate the accuracy and robustness of the present computational framework.

Fig. 16 A and B present a comparison between the experimentally observed [97] and numerically predicted melt pool morphologies across the eight validation cases. The results reveal distinct flow regimes driven by the processing parameters. In Cases III–V, characterized by lower scanning speeds, the melt pool exhibits a *keyhole mode*. Here, the model successfully captures the localized expansion and deep penetration caused by multiple internal reflections of the laser beam within the vapor depression. Conversely, as the scanning speed increases, the melt pool transitions into a *conduction mode*, becoming shallower and more elongated. The proposed ray-tracing model accurately reproduces these

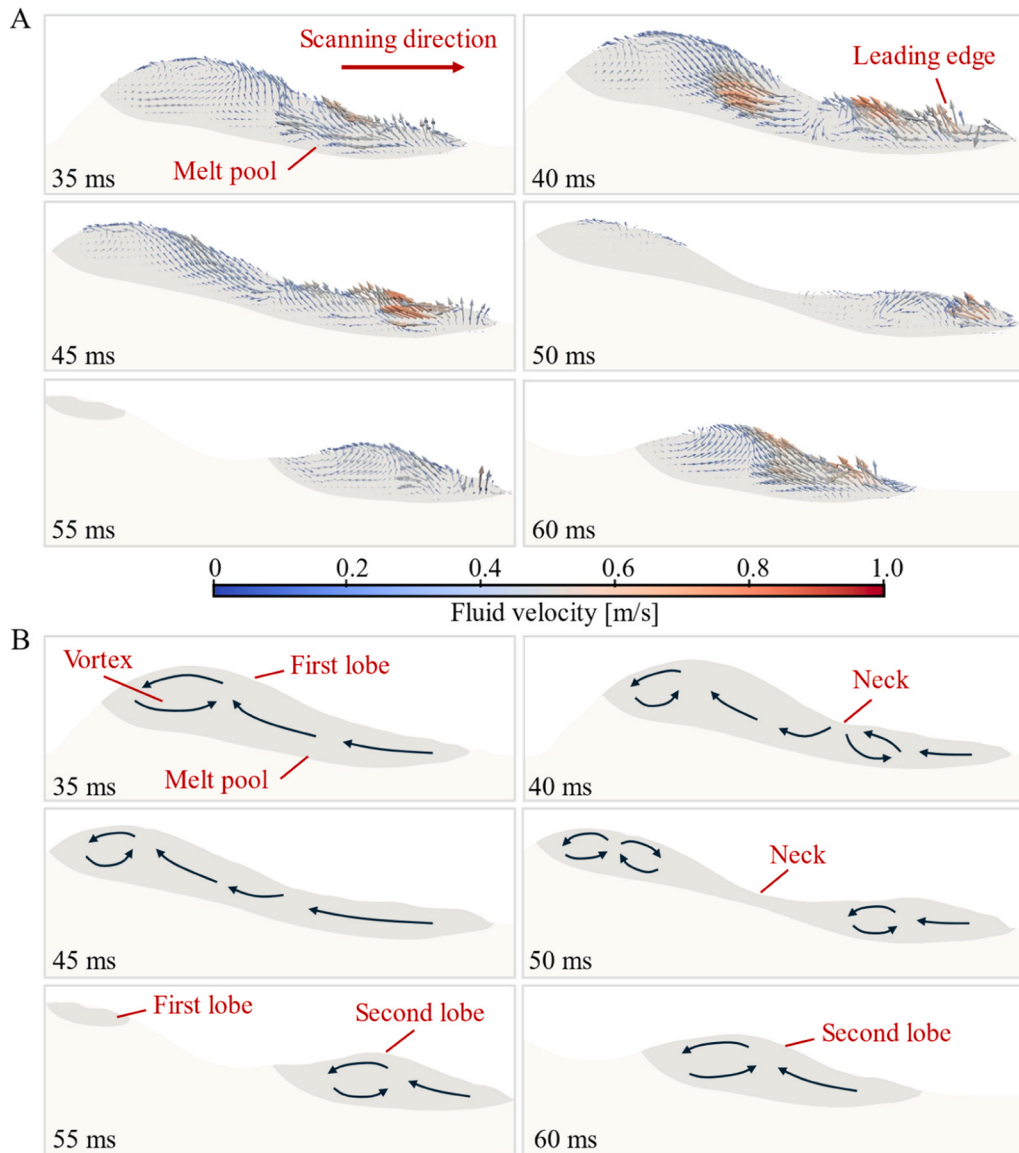


Fig. 15. Simulated results for a contact angle of 150° at six time instants: (A) velocity field along section A-A, and (B) schematic of melt-pool flow patterns along section A-A. Note: the position of section A-A is illustrated in Fig. 13 A.

geometric transitions, demonstrating its capability to capture the complex laser-matter interactions across a broad process window.

To quantify the model's accuracy, the simulated melt pool depth and the tangent of the front wall angle are compared against empirical linear correlations derived from extensive experiments [97] (Fig. 16 C and D). The simulation results show excellent agreement with the experimental data across all eight cases, which were strategically selected to cover a wide spectrum of energy densities. Quantitatively, the root-mean-square errors (RMSE) of the predicted keyhole depth obtained from the eight cases in Fig. 16 C and Fig. 16D are approximately 4.2 μm and 6.5 μm , respectively. These values correspond to about 2.4% and 3.7% of the average keyhole depth (175.5 μm), indicating that the deviations remain within an acceptable error range. The remaining discrepancies may be attributed to several modeling simplifications, such as the absence of an explicitly resolved high-velocity vapor jet. Crucially, the minor discrepancies observed fall well within the reported experimental error margins [97]. This robust quantitative agreement provides strong evidence for the validity of the present ray-tracing formulation in predicting precise melt pool morphologies.

3.3.2. Powder stream heating

This study extends the validation to the PB-DED process regime, where the interaction between the laser beam and the dynamic powder stream is critical. A second benchmark case was established based on the experimental setup reported in Ref. [37]. The configuration features two convergent powder streams inclined at 20°, injected from a nozzle with a 10 mm tip diameter. These streams intersect at the laser focal plane, where in-flight particle temperatures were experimentally measured. The feedstock material is AISI 304 stainless steel, with simulation parameters detailed in Table E.4. The particles are modeled as uniform spheres with a radius of 45 μm , an initial temperature of 60 °C, and a mean velocity of 1.38 m/s. The laser beam radius is set to 0.75 mm, and three distinct power levels, 500 W, 800 W, and 1000 W, were evaluated.

To investigate the effects of particle distribution density, two representative simulation scenarios were constructed. Case I (Fig. 17 A) represents an idealized sparse stream, where each nozzle releases a single particle per time step with a minor random positional offset (within one particle diameter). In this regime, inter-particle collisions are negligible, and heating is dominated by direct laser irradiation. In contrast, Case II (Fig. 17 C) mimics realistic high-density nozzle

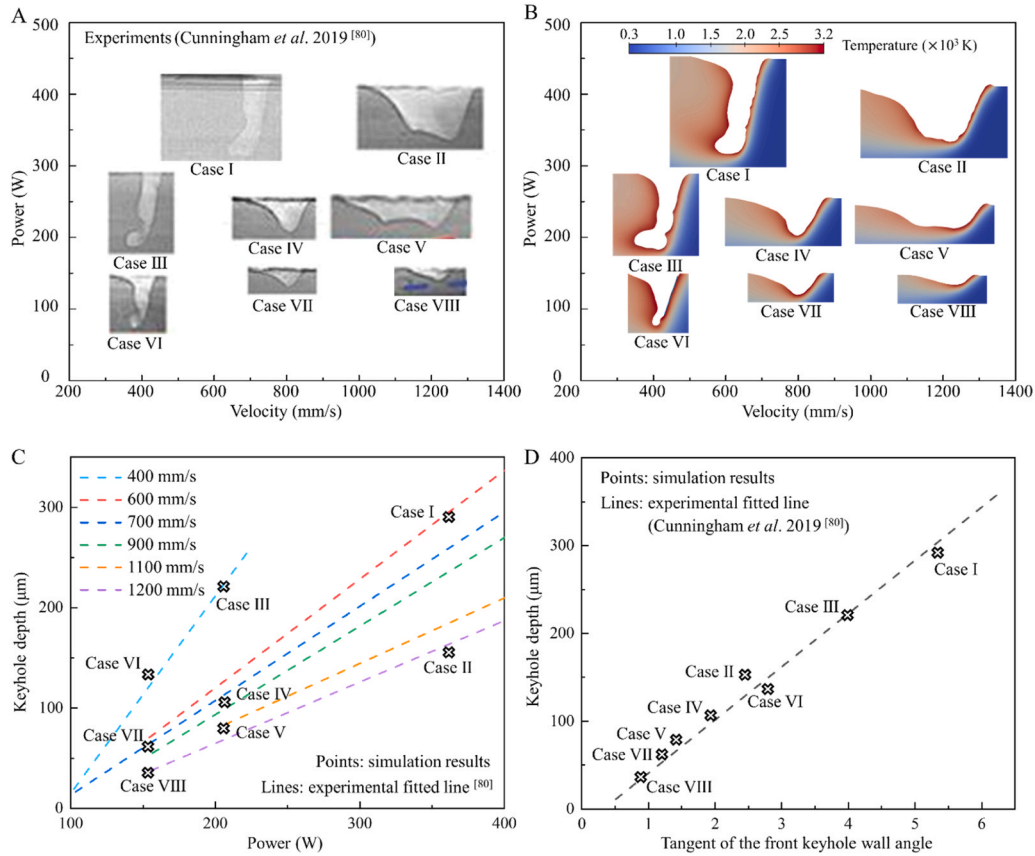


Fig. 16. Comparison between experimental [97] and simulated results for the validation of the proposed ray-tracing model. (A) Experimental melt pool morphologies under different laser powers and scanning speeds. (B) Simulated melt pool morphologies under the same conditions. (C) Comparison of melt pool depths from experiments and simulations with the experimentally fitted line [97] versus laser power. (D) Comparison of the tangent of the front keyhole wall angle versus keyhole depth between experimental [97] and simulated results for all eight cases (Table E.3).

behavior. Here, each stream emits five particles per interval with varying velocity vectors, generating a dispersed cloud. This configuration accounts for stochastic inter-particle collisions prior to reaching the focal zone, resulting in a spatially irregular distribution that significantly alters the optical path.

Fig. 17B and D quantify the temporal evolution of the average particle temperature at the focal plane. Given the stochastic nature of injection and collision dynamics, the temperature was averaged over a control volume centered at the theoretical intersection point. The sampling domain was defined as $400 \mu\text{m} \times 400 \mu\text{m} \times 600 \mu\text{m}$ in the x, y, and z directions, respectively. The constrained dimensions in the x and y directions serve to exclude artifacts from substrate rebound, while the extended z-dimension ensures a sufficient sample size for statistically robust averaging.

A comparative analysis of Fig. 17B and D reveals that Case I exhibits relatively stable thermal histories, consistent with its simplified, collision-free nature. Conversely, Case II displays significant temporal fluctuations. Quantitatively, the standard deviations of particle temperature for Case I are 25.7 K, 33.9 K, and 42.7 K across the three power levels. In Case II, these values rise sharply to 74.4 K, 117.1 K, and 105.2 K, approximately a two- to threefold increase. This substantial variance in the realistic case highlights the impact of complex optical phenomena, including mutual shadowing, multi-scattering, and the stochasticity of particle trajectories, on local thermal variability.

Notwithstanding these instantaneous fluctuations, the time-averaged particle temperature exhibits statistical convergence, accurately reflecting the net energy absorption of the powder stream. As summarized in Table 1, the simulated average temperatures at the focal plane show excellent agreement with experimental measurements, with a

maximum relative deviation of less than 5%. This high level of concordance confirms the fidelity of the proposed ray-tracing framework in capturing the intricate thermodynamics of laser-powder interactions under realistic PB-DED conditions.

3.4. Validation of PB-DED

Having independently validated the constituent modules of the proposed methodology, we proceeded to perform a full-scale PB-DED simulation to comprehensively assess the integrated performance of the multi-phase semi-resolved CFD-DEM framework. In PB-DED, the final morphology of the deposited melt track is a cumulative result of complex multi-physics interactions and serves as a critical metric for the model's predictive fidelity. In this section, numerical simulations are conducted and benchmarked against the experimental data reported in Ref. [37] (employing the same experimental setup detailed in Section 3.3.2). Four representative cases, spanning various combinations of laser power, scanning speed, and powder mass flow rate, were selected for validation, as summarized in Table E.5.

The substrate and feedstock material employed is AISI 304 stainless steel, with thermophysical properties listed in Table E.4. For this specific benchmark, metal evaporation is neglected; consequently, vaporization-related parameters are excluded. The powder injection configuration follows the schematic in Fig. 17 A, featuring two powder streams inclined at 20° relative to the z-axis. Regarding the optical focal plane, as the exact position was not specified in the reference experiment, it is assumed to coincide with the substrate top surface to maximize powder catchment efficiency. The powder mass flow rate is regulated by the particle injection frequency; for example, a rate of 4 g/min is achieved

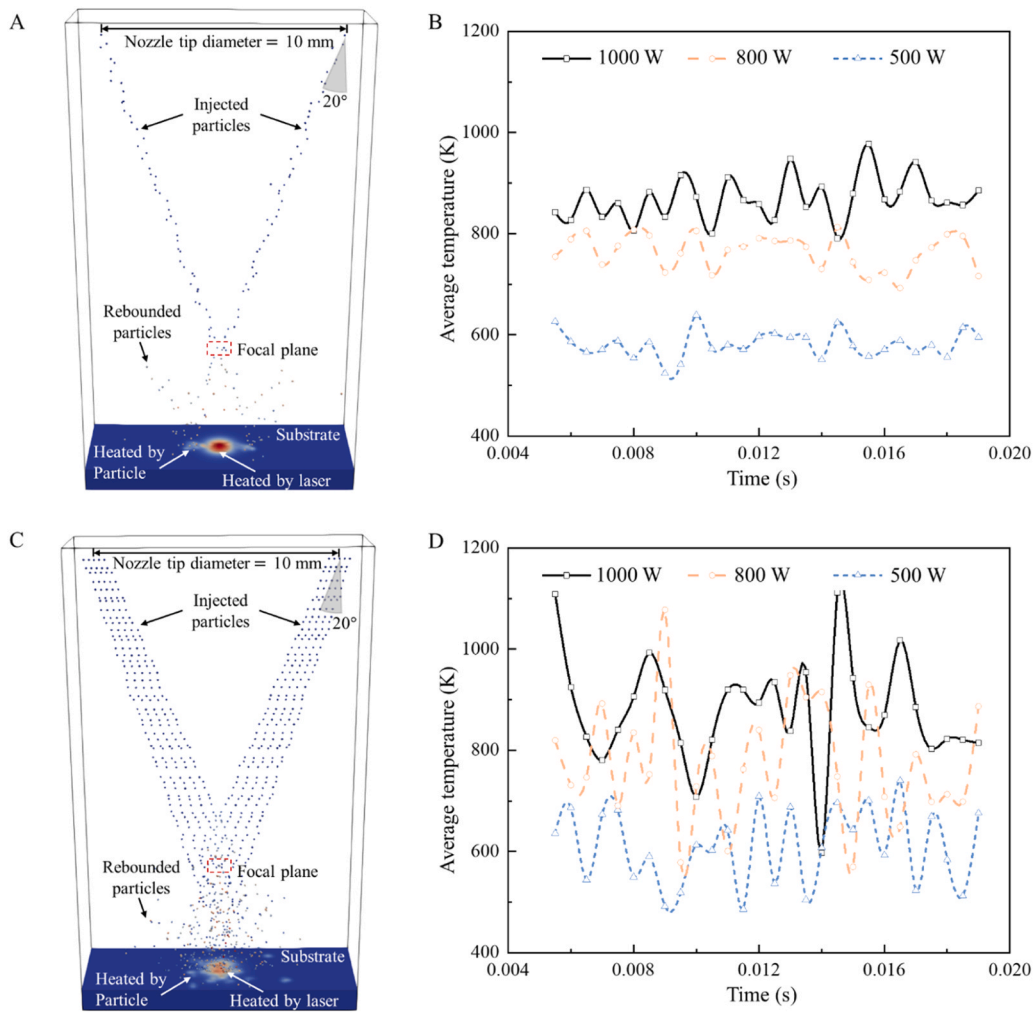


Fig. 17. (A and C) Numerical models of powder stream heating for Case I (A) and II (C); (B and D) Simulated temperature of powder particles at the focal plane under three laser energy levels (500, 800, and 1000 W) for Case I (B) and II (D).

Table 1

Comparison of experimental [37] and numerical results for powder stream heating.

Laser power [W]	Temperature of powder particles at the focal plane			
	Experiment results [°C] [37]	Simulation results [°C]		Error [%]
		Case I	Case II	
500	321.22	308.04	313.46	4.1
800	488.61	493.32	502.28	1.0
1000	608.81	595.62	606.65	2.2

by injecting four particles every 165 μ s.

The computational domain encompasses a volume of $10 \times 6 \times 5.5 \text{ mm}^3$. To balance accuracy and computational cost, an adaptive mesh refinement (AMR) strategy was implemented: a background grid size of 100 μ m was used for the far field, while a refined grid of 50 μ m was locally applied to the melt track and the substrate interface region. The particle radius was fixed at 45 μ m. Temporal discretization was governed by the CFL criterion, with the Courant number capped at 0.5. To ensure numerical stability, a hard ceiling of 50 μ s was imposed on the time step, with the actual step size being the minimum of the CFL-derived value and this limit. The solid-liquid contact angle was calibrated based on the experimental wetting profiles (Fig. 18 C and D) and

was prescribed as 30° for these simulations. Details of the convergence study based on Case I are provided in Appendix F.

Fig. 18A and B depict the simulated melt track morphologies for Case I and Case IV, respectively. For rigorous validation, cross-sectional profiles were extracted at $x = 5.5 \text{ mm}$ from both the simulations and the corresponding experiments (Fig. 18 C and D). While experimental cross-sections were available only for these two cases, the simulated cross-sections for all cases are documented. Table 2 summarizes the quantitative evaluation of three key geometric parameters: height above substrate (h_1), remelted depth (h_2), and maximum width (d), as defined schematically in Fig. 18D.

The quantitative comparisons reveal that the melt track geometry is highly sensitive to process parameters. For instance, decreasing the scanning speed from 1000 mm/s (Case I) to 500 mm/s (Case II) results in a near-doubling of the melt pool height, from 0.182 mm to 0.354 mm. The proposed numerical framework successfully captures these non-linear dependencies, exhibiting excellent agreement with experimental measurements. The relative discrepancy between simulated and experimental results remains within approximately 5% across all metrics. Such deviations may partially originate from unavoidable uncertainties in the experimental conditions, as well as modeling simplifications adopted in the present study. In particular, the exact laser intensity distribution of the experimental system is not available. Therefore, a commonly used Gaussian beam profile was assumed in the ray-tracing model, which may introduce minor differences in the predicted energy deposition. This high level of accuracy confirms the applicability of the

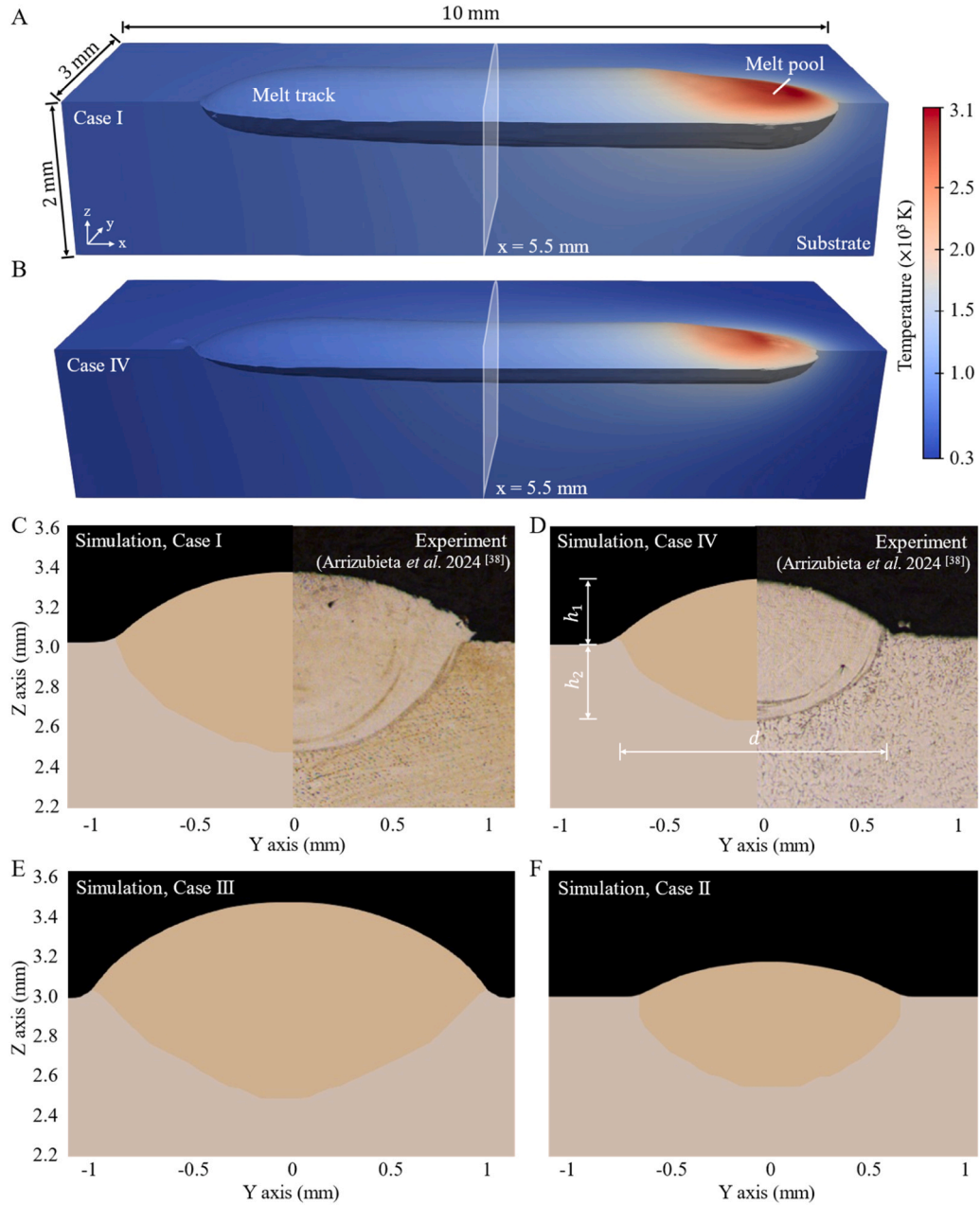


Fig. 18. Comparison of simulated and experimental melt tracks [37]: surface morphology for Case I (A, C) and Case IV (B, D); cross-sectional profiles for Case III (E) and Case II (F). All cross-sections (C-F) are extracted at $x = 5.5$ mm, as indicated in (A, B), and are aligned along a common y-axis.

Table 2

Comparison of experimental [37] and numerical results for melt track morphology.

Case	Experimental results [mm] [37]			Simulation results [mm]			Absolute error [%]		
	h_1	$h_1 + h_2$	d	h_1	$h_1 + h_2$	d	h_1	$h_1 + h_2$	d
I	0.354	0.936	1.663	0.349	0.899	1.646	1.41	3.98	1.02
II	0.182	0.614	1.351	0.175	0.625	1.300	3.85	1.79	3.77
III	0.484	0.992	1.869	0.481	0.981	1.967	0.62	1.11	5.24
IV	0.283	0.717	1.441	0.291	0.741	1.500	2.82	3.23	3.93

algorithm for predicting deposit morphology in PB-DED processes. Critically, the predictive fidelity of the full-scale simulation is a direct consequence of the accurate resolution of the underlying sub-processes validated in Sections 3.1–3.3, specifically, the precise coupling of particle-laser heating (Fig. 17, Table 1) and the robust hydrodynamics of the melt pool (Fig. 16).

4. Illustrative simulations

4.1. Model setup

Accurate simulation of large-scale PB-DED processes is critical for advancing their industrial applications, as it enables the prediction and

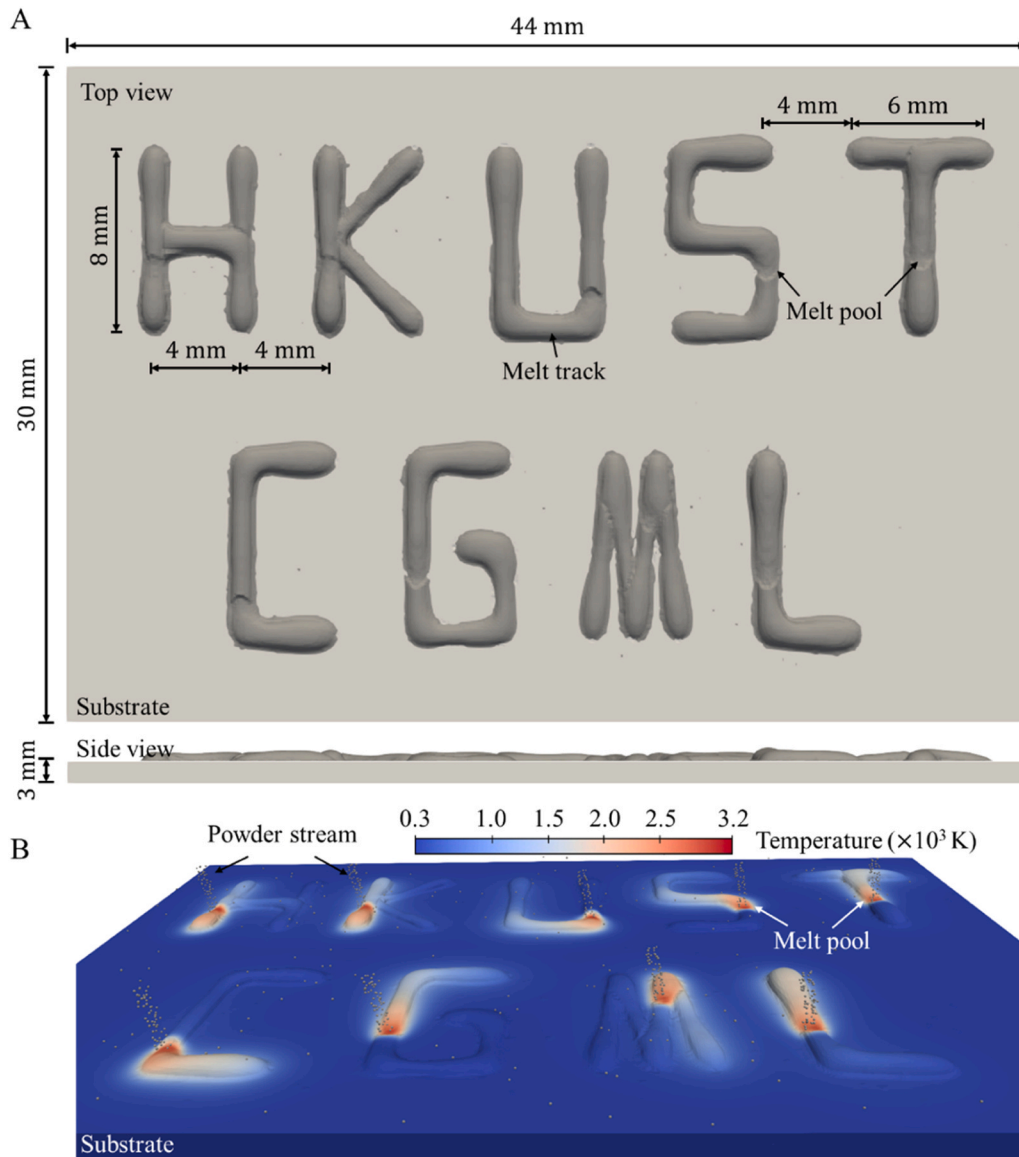


Fig. 19. Schematic diagram of the illustrative simulation setup: (A) Top and front views of the nine-letter logo with dimensional annotations; (B) Distribution of the temperature field and powder streams in the model.

mitigation of defects, the optimization of process parameters, and a deeper understanding of the complex multi-physics phenomena involved. To further demonstrate the capability of the proposed algorithm in handling large-scale PB-DED applications, including multi-laser, multi-powder-stream, multi-layer, and multi-track scenarios, this chapter presents an illustrative case study that simulates the printing of our laboratory's lettered logo: "HKUST CGML."¹ Fig. 19 A illustrates the layout of the nine letters. Except for the letter "T", which has a width of 6 mm, all other letters are 4 mm wide, while the height of every letter is 8 mm. The letters are arranged in two rows separated by a 6 mm gap, with a 4 mm spacing between adjacent letters within the same row. Each of the nine letters is printed independently using a single-sided powder feeding configuration, which accordingly employs nine powder streams and nine laser beams (Fig. 19B). During the actual printing process, for each letter, the powder streams and laser beams are continuously moved from a starting point until the entire letter is completed. The scanning

speed is set to 0.1 m/s for letters with non-repeating strokes (e.g., U, S, L) and increased to 0.2 m/s for letters containing overlapping or repeated strokes (e.g., T, H). The powder material used is Ti-6Al-4V, with material properties provided in Table E.1 and Table E.2. The powder particles have diameters of 80 μm , 90 μm , and 100 μm , with a proportional distribution of 0.3, 0.4, and 0.3, respectively. The initial temperature of both the computational domain and the powder particles is set to 300 K. A fixed temperature boundary of 300 K is also imposed at the bottom of the substrate. The substrate thickness is set to 3 mm, which is approximately twice the characteristic size of the laser interaction region. According to the simulation results, the temperature at the substrate surface about 3 mm away from the laser center is only around 315 K. Therefore, the 3 mm substrate thickness is considered sufficient to minimize the influence of the bottom boundary condition while maintaining computational efficiency.

Each laser beam has a radius of 0.75 mm and a power of 1000 W, with a Gaussian energy distribution. The computational domain measures 44 mm $\times$ 30 mm $\times$ 4 mm. An adaptive mesh refinement technique is applied, with a background grid size of 200 μm and a refined grid size of 100 μm . In this simulation, the number of refined grids ranges

¹ Here, "HKUST" stands for the Hong Kong University of Science and Technology, and "CGML" denotes the Computational Granular Mechanics Laboratory.

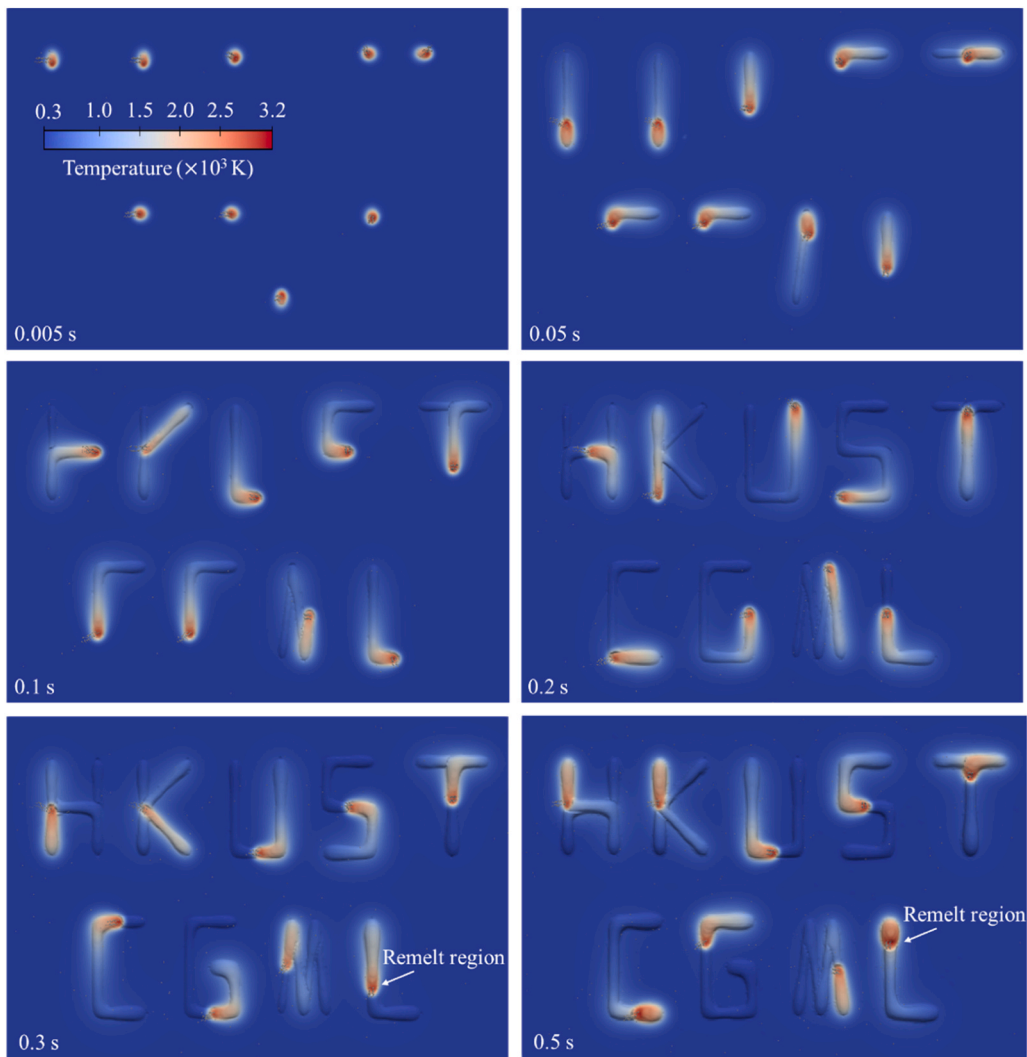


Fig. 20. Snapshots of the temperature field and melt track morphology at different time instants: 0.005 s, 0.05 s, 0.1 s, 0.2 s, 0.3 s, and 0.5 s.

between 1.6 million and 2.0 million, depending on the length of the melt track. The time step is adaptively controlled by the Courant-Friedrichs-Lewy (CFL) condition, with a maximum CFL number of 0.5. To ensure numerical accuracy, the time step is capped at 50 μ s. Under the above settings, simulating 0.5 s of the physical process required approximately 9 h of computation time on an NVIDIA GeForce RTX 5070 GPU. The memory consumption of the present approach was observed to be approximately 2 GB per million grid cells.

In contrast, a traditional fully resolved approach would require explicitly resolving the flow field around every individual powder particle, resulting in a mesh density at least 512 times larger than that used in the present semi-resolved model for the same computational domain. Consequently, the fully resolved method would lead to a prohibitive memory requirement exceeding 1 TB, which is far beyond the capacity of typical single-GPU workstations. By comparison, the proposed semi-resolved framework completes the same simulation using less than 16 GB of GPU memory, demonstrating its substantial advantage in computational efficiency.

4.2. Simulation results

Fig. 20 illustrates the printing process of the logo, where each laser and powder stream is dedicated to an individual letter, which moves at predefined speeds in a periodic, multi-layer deposition pattern. Notably, upon completing the first layer of a letter, its trajectory reverses to

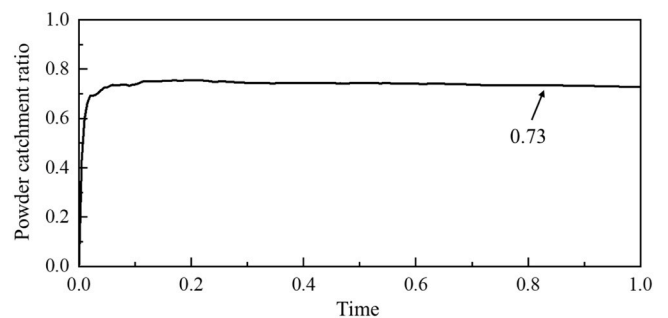


Fig. 21. Temporal evolution of powder catchment ratio, defined as the ratio of incorporated powder to injected powder.

return the laser and powder stream to the starting point before repeating the motion. For instance, as shown in Fig. 20, the letter T undergoes its initial forward printing between 0 s and 0.1 s, followed by a reverse printing phase, as observed at 0.2 s. By 0.3 s, the letter T has entered its second full printing cycle. The direction of laser movement can be inferred from the temperature distribution along the melt track. For example, at 0.3 s and 0.5 s, the melt pool position in the letter U appears nearly identical. However, the thermal gradient along the adjacent melt track is reversed, indicating opposite scanning directions and forward at

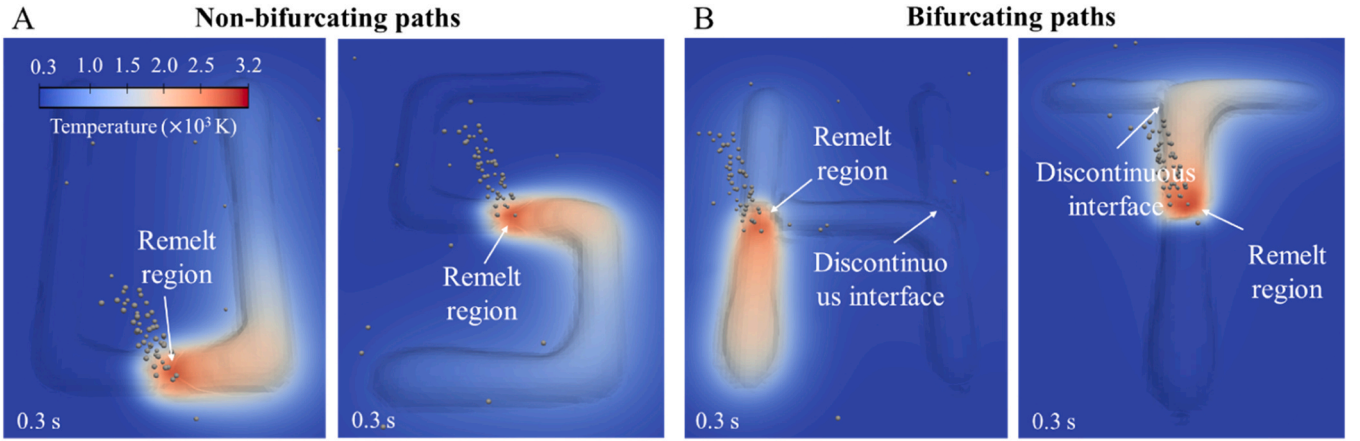


Fig. 22. Comparison of melt pool morphology and temperature distribution for (A) non-bifurcating paths (letters U and S) and (B) bifurcating paths (letters H and T).

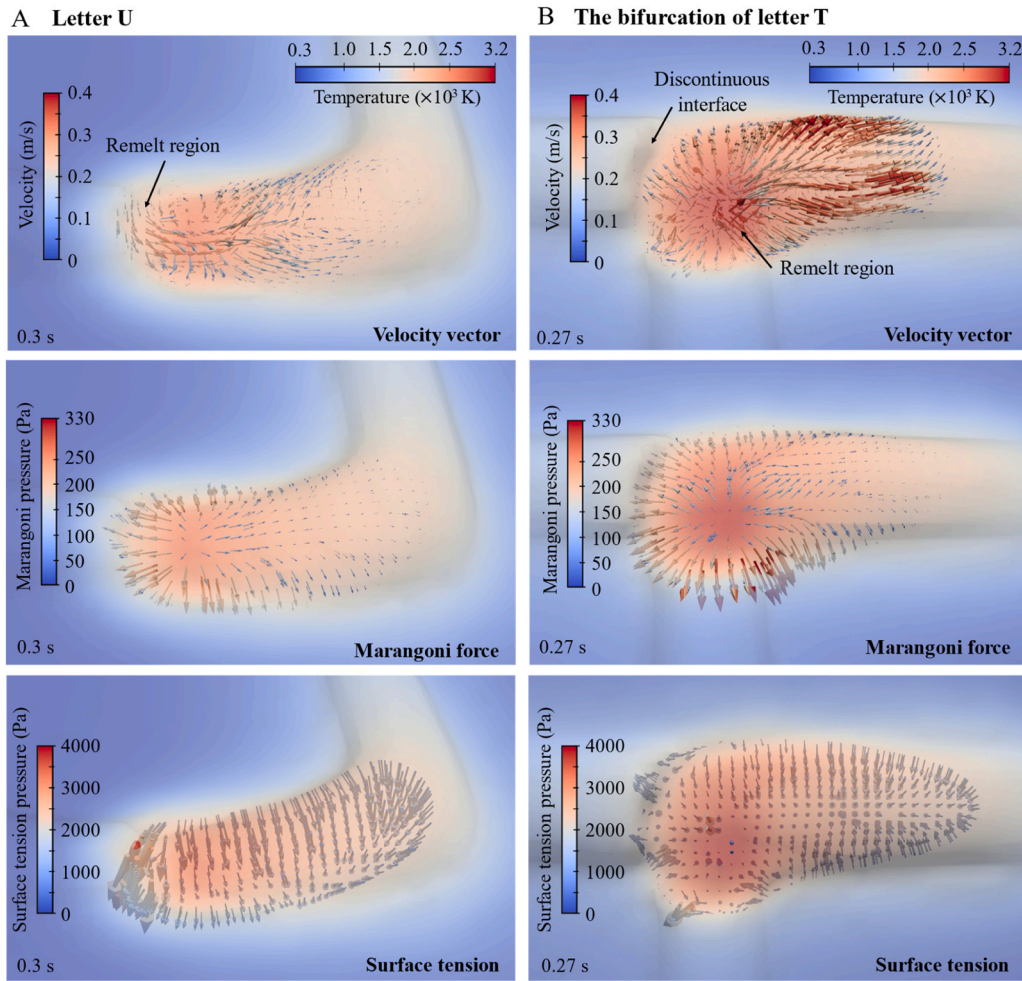


Fig. 23. Melt pool characteristics for different geometric features: temperature field, velocity vectors, and Marangoni force in the letter U (A) and at the bifurcation of the letter T (B). The color on the metal surface represents the temperature field, while the arrows indicate vector quantities (e.g., velocity or force), with the arrow color corresponding to their magnitudes.

0.3 s and reverse at 0.5 s.

Fig. 21 presents the time evolution of the powder catchment ratio, defined as the ratio of incorporated powder to injected powder. This metric highlights a key advantage of the CFD-DEM framework, namely its capability to directly quantify powder utilization efficiency during the deposition process. At the initial stage, before melting occurs, most

particles impinge on the substrate and rebound, resulting in a negligible catchment ratio. As laser heating is applied and melting initiates, particles increasingly enter and are captured by the melt pool, leading to a gradual increase in the powder catchment ratio. Due to the stochastic nature of particle injection, fluctuations are observed in the early stage. Over time, the system reaches a quasi-steady state, with the powder

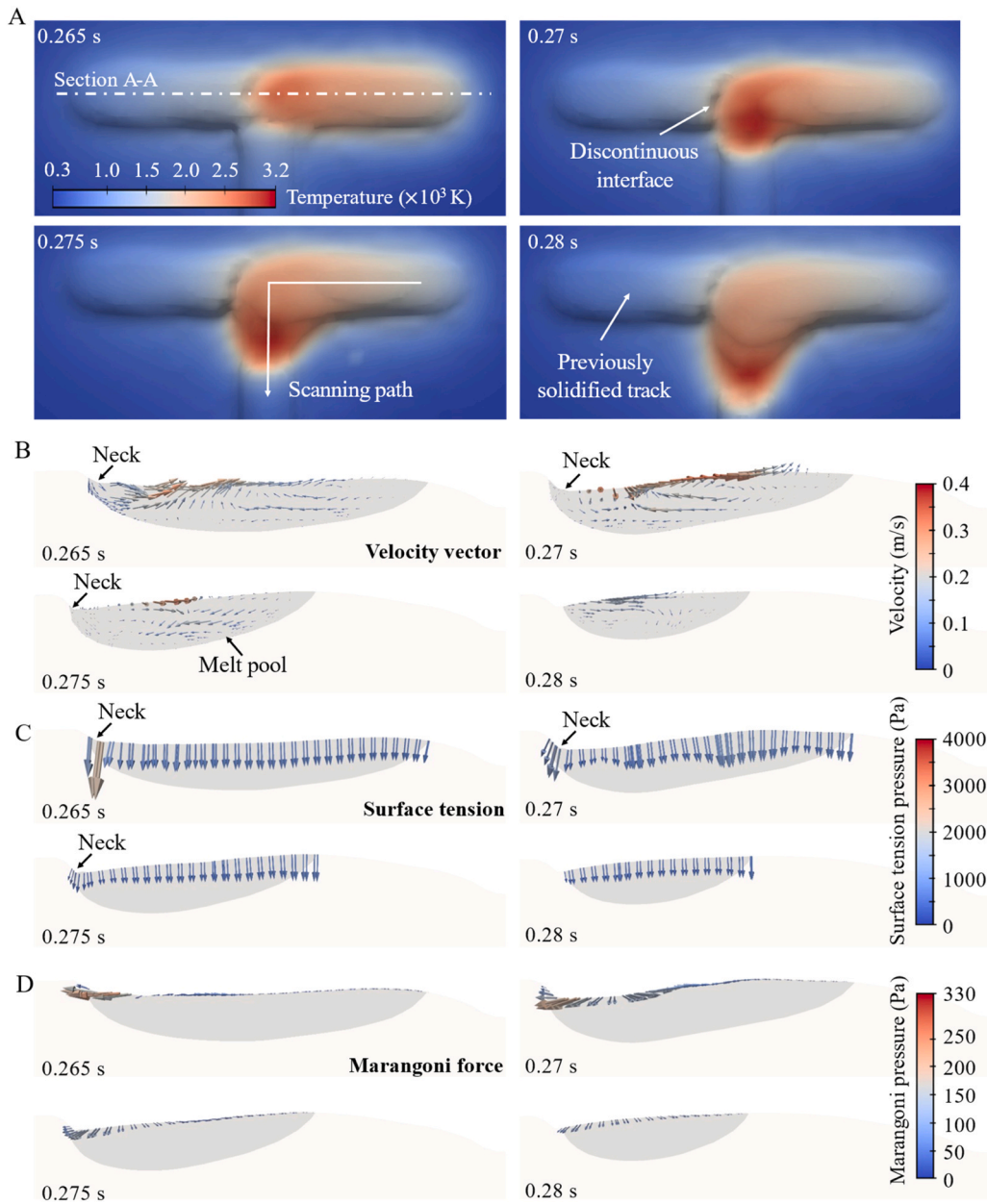


Fig. 24. Transient melt pool characteristics during T-shaped scanning: temperature field (A), cross-sectional velocity vectors (B), surface tension (C), and Marangoni forces (D). Note that the results in (B)–(D) are presented on the cross-section A–A indicated in (A). It is important to clarify that while the Marangoni forces (D) appear to have normal components in this 2D projection, they are physically defined as shear stresses acting tangentially to the 3D free surface. The apparent downward inclination is a geometric artifact resulting from intersecting the curved 3D surface vectors with the 2D cross-sectional plane.

catchment ratio stabilizing at approximately 0.73.

Further analysis of the simulation results at 0.3 s and 0.5 s reveals that remelting leads to visible discontinuities in the melt track. Here, the remelt region is defined as an area where previously solidified material is reheated and melted again due to subsequent powder deposition and laser interaction. To systematically investigate this behavior, letters are categorized into two types based on path geometry: non-bifurcating and bifurcating. Fig. 22 presents magnified views of these two categories during printing. In non-bifurcating letters (Fig. 22 A), discontinuities are primarily observed in remelt regions but tend to diminish with further deposition. In contrast, for bifurcating letters (Fig. 22B), a discontinuous interface forms at path intersections in addition to remelt-induced gaps. This interface persists after solidification, resulting in a distinct boundary. This occurs because the remelted original track and the newly formed melt flow, influenced by surface tension and contact angle

effects, merge into a hemispherical melt track similar to that shown in Fig. 9. The resulting geometry produces a discontinuous interface with the intersecting track.

Fig. 23 further depicts the velocity vector, Marangoni force and surface tension distributions in the melt pool of letter U and at the bifurcation of letter T, respectively. First, the overall trends of the velocity field show high consistency with the distributions of Marangoni force and surface tension. It is observed that the molten fluid near the laser center predominantly flows opposite to the scanning direction. Regarding the driving forces, the Marangoni force vector points radially outward from the laser center, driven by the negative temperature coefficient of surface tension and the peak temperature at the center. Conversely, the surface tension acts perpendicular to the melt pool surface, pointing almost exclusively inward. It is worth noting that the surface tension at the melt pool boundaries is significantly intensified,

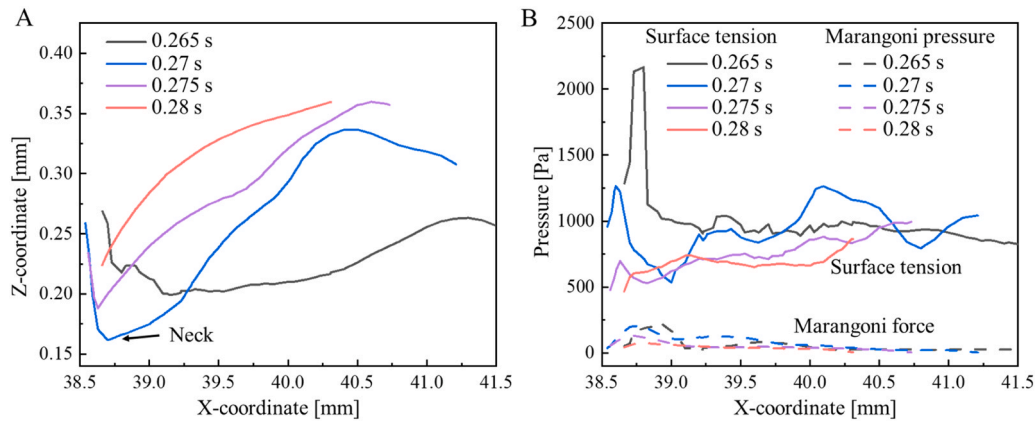


Fig. 25. Quantitative profiles along the cross-section A-A: (A) variation of the z-coordinate (interface height) along the x-axis; and (B) distributions of surface tension and Marangoni pressure.

reaching magnitudes up to twice those found in the pool center. Furthermore, a quantitative comparison of the two forces indicates that the equivalent pressure generated by surface tension (Laplace pressure) is 5–10 times greater than the Marangoni pressure, highlighting its dominant role in maintaining the melt pool morphology.

To elucidate the formation mechanism of the discontinuous interface at the bifurcation, the temporal evolution of the melt pool morphology, along with the velocity, surface tension, and Marangoni force fields for the letter T, are analyzed at four distinct moments, as shown in Fig. 24. Additionally, Fig. 25 provides a quantitative correlation between the interface profile and the driving forces. These moments capture the dynamic transition of the melt pool during the turning process, where the surface morphology evolves from significant fluctuation to a stable smooth arc. At $t = 0.265$ s, immediately prior to the laser entering the bifurcation zone, the molten fluid exhibits a strong backward convection consistent with Fig. 23, initially triggered by Marangoni shear stresses. This continuous backward mass transport leads to the formation of a "neck" at the leading edge. A critical observation from Fig. 25 is the magnitude of the surface tension pressure in this neck region, which peaks at approximately 2165 Pa. This dominant capillary force squeezes the fluid downward, significantly intensifying the backward flow. While the Marangoni force attempts to counteract this capillary-driven flow, its magnitude is insufficient, ranging from only 10% to 20% of the surface tension pressure, confirming that surface tension is the governing force in the necking phenomenon.

Subsequently, as the laser proceeds away from the bifurcation, the local solidification front advances on the left side of the neck (near the pre-existing track), causing the neck geometry to vanish from the cross-section of the melt pool. Although the force fields homogenize during this phase, the surface tension remains dominant (exceeding the Marangoni force by a factor of at least two). This force balance dictates a convex equilibrium shape, constraining lateral spreading. The solidification of this transient flow structure ultimately manifests as the observed discontinuous interface in the solidified track.

This illustrative case, involving the printing of nine letters with varying path geometries, demonstrates the capability of the proposed method to simulate large-scale PB-DED processes. It successfully handles complex scanning paths, multi-layer and multi-track deposition, and the interaction of multiple laser and powder beams. Beyond numerical robustness, the framework provides deep physical insights into the competitive mechanisms between capillary and thermocapillary forces. These insights are pivotal for practical engineering applications, offering a predictive basis for tailoring scanning patterns to counteract surface tension-driven instabilities, thus ensuring high part quality even in components with intricate topological features.

5. Conclusions and outlooks

In this work, we have established a comprehensive, high-fidelity computational framework for powder-based directed energy deposition (PB-DED) by unifying a semi-resolved CFD-DEM coupling with a sophisticated multi-physics laser-matter interaction model. The proposed methodology successfully bridges a critical gap in the simulation landscape, enabling the simultaneous resolution of powder-scale dynamics and continuum-scale melt pool evolution, which is essential for predicting mesoscale defect formation in PB-DED.

The core achievements of this study are threefold. First, an existing kernel-based semi-resolved CFD-DEM framework is adapted and extended for PB-DED processes, and systematically assessed to demonstrate that it provides an effective balance between computational efficiency and physical fidelity at relevant length scales. This is achieved by incorporating problem-specific physical models, including particle collision dynamics, phase change behavior, and a VOF-compatible ray-tracing laser model, enabling a physically consistent treatment of laser energy deposition on both discrete particles and the diffuse melt pool interface within a unified framework. Second, the framework's predictive capability is verified across a range of coupled phenomena, including particle transport, contact-angle-driven wetting, and laser heating of both bare substrates and powder streams, showing good agreement with available experimental data. Furthermore, the model provides mechanistic insights into key process instabilities, including the balling effect and the formation of discontinuous interfaces induced by bifurcating paths in multi-track and multi-layer deposition, highlighting its potential for improved understanding of defect formation and for supporting process optimization in PB-DED. Third, by re-designing the entire computational pipeline for GPU architectures, the proposed approach enables large-scale, high-resolution simulations of complex multi-laser, multi-track, and multi-layer deposition processes on cost-effective hardware, significantly improving computational efficiency. An illustrative multi-track simulation further demonstrates the capability of the framework and suggests its potential for extension to realistic engineering-scale applications.

While the current model offers a powerful foundation, future work will focus on incorporating more granular physics, including the explicit modeling of nozzle gas flow, the temperature-dependent evolution of contact angles, and the effects of partial particle melting in-flight. These enhancements will further solidify the framework's role as a cornerstone for the next generation of predictive, optimized, and intelligent metal additive manufacturing processes.

Author Statement

We declare that this manuscript is original, has not been published

before and is not currently being considered for publication elsewhere.

We confirm that the manuscript has been read and approved by all named authors and that there are no other persons who satisfied the criteria for authorship but are not listed. We further confirm that the order of authors listed in the manuscript has been approved by all of us.

We understand that the Corresponding Author is the sole contact for the Editorial process. He is responsible for communicating with the other authors about progress, submissions of revisions and final approval of proofs.

CRedit authorship contribution statement

Jidong Zhao: Writing – review & editing, Supervision, Funding acquisition. **Tao Yu:** Writing – original draft, Visualization, Validation, Software, Methodology, Formal analysis. **Yong Kong:** Writing – original draft, Visualization.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgments

This work was financially supported by National Natural Science Foundation of China (Key Project #52439001) and Research Grants Council of Hong Kong (GRF 16203123, 16208224, CRF C7085–24G, RIF R6008–24, YCRF C6002–24Y, and TRS T22–607/24 N).

Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at [doi:10.1016/j.addma.2026.105288](https://doi.org/10.1016/j.addma.2026.105288).

Data availability

Data will be made available on request.

References

- [1] J. Kelly, J. Elmer, F. Ryerson, J. Lee, J. Haslam, Directed energy deposition additive manufacturing of functionally graded Al-W composites, *Addit. Manuf.* 39 (2021) 101845.
- [2] C.-Y. Wu, M.-C. Lu, W.-C. Yang, N.-C. Chi, Experimental study of balling defect generation and audible sound analysis in directed energy deposition metal additive manufacturing, *The, Int. J. Adv. Manuf. Technol.* 134 (2024) 205–221.
- [3] N. Shamsaei, A. Yadollahi, L. Bian, S.M. Thompson, An overview of Direct Laser Deposition for additive manufacturing; Part II: mechanical behavior, process parameter optimization and control, *Addit. Manuf.* 8 (2015) 12–35.
- [4] H. Liu, Z. Hu, X. Qin, Y. Wang, J. Zhang, S. Huang, Parameter optimization and experimental study of the sprocket repairing using laser cladding, *The, Int. J. Adv. Manuf. Technol.* 91 (2017) 3967–3975.
- [5] Z. Liu, B. He, T. Lyu, Y. Zou, A review on additive manufacturing of titanium alloys for aerospace applications: directed energy deposition and beyond Ti-6Al-4V, *Jom* 73 (2021) 1804–1818.
- [6] M.-P. Hong, W.-S. Kim, J.-H. Sung, D.-H. Kim, K.-M. Bae, Y.-S. Kim, High-performance eco-friendly trimming die manufacturing using heterogeneous material additive manufacturing technologies, *Int. J. Precis. Eng. Manuf. -Green. Technol.* 5 (2018) 133–142.
- [7] A. Saboori, A. Aversa, G. Marchese, S. Biamino, M. Lombardi, P. Fino, Application of directed energy deposition-based additive manufacturing in repair, *Appl. Sci.* 9 (2019) 3316.
- [8] W. Harun, M. Kamariah, N. Muhamad, S. Ghani, F. Ahmad, Z. Mohamed, A review of powder additive manufacturing processes for metallic biomaterials, *Powder Technol.* 327 (2018) 128–151.
- [9] D.J. Ryu, H.Y. Ban, E.Y. Jung, C.-H. Sonn, D.H. Hong, S. Ahmad, B. Gweon, D. Lim, J.H. Wang, Osteo-compatibility of 3D titanium porous coating applied by direct energy deposition (DED) for a cementless total knee arthroplasty implant: in vitro and in vivo study, *J. Clin. Med.* 9 (2020) 478.
- [10] T. DeRoy, H.L. Wei, J.S. Zuback, T. Mukherjee, J.W. Elmer, J.O. Milewski, A. M. Beese, Ad Wilson-Heid, A. De, W. Zhang, Additive manufacturing of metallic components—process, structure and properties, *Progress. Mater. Sci.* 92 (2018) 112–224.
- [11] W.E. Frazier, Metal additive manufacturing: a review, *J. Mater. Eng. Perform.* 23 (2014) 1917–1928.
- [12] S.K. Everton, M. Hirsch, P. Stravroulakis, R.K. Leach, A.T. Clare, Review of in-situ process monitoring and in-situ metrology for metal additive manufacturing, *Mater. & Des.* 95 (2016) 431–445.
- [13] M. Grasso, B.M. Colosimo, Process defects and in situ monitoring methods in metal powder bed fusion: a review, *Meas. Sci. Technol.* 28 (2017) 044005.
- [14] Y. Huang, M.B. Khamesee, E. Toyserkani, A comprehensive analytical model for laser powder-fed additive manufacturing, *Addit. Manuf.* 12 (2016) 90–99.
- [15] Y. Javid, M. Ghoreishi, Thermo-mechanical analysis in pulsed laser cladding of WC powder on Inconel 718, *Int. J. Adv. Manuf. Technol.* 92 (2017) 69–79.
- [16] Y. Lee, D. Farson, Surface tension-powered build dimension control in laser additive manufacturing process, *Int. J. Adv. Manuf. Technol.* 85 (2016) 1035–1044.
- [17] D. Rommel, M. Terock, F. Scherm, C. Kuttner, U. Glatzel, Direct metal deposition of abrasive tracks—Potentials concerning geometry and materials, *J. Laser Appl.* 29 (2017).
- [18] H.-W. Hsu, Y.-L. Lo, M.-H. Lee, Vision-based inspection system for cladding height measurement in Direct Energy Deposition (DED), *Addit. Manuf.* 27 (2019) 372–378.
- [19] D.S. Ertay, M.A. Naiel, M. Vlasea, P. Fieguth, Process performance evaluation and classification via in-situ melt pool monitoring in directed energy deposition, *CIRP J. Manuf. Sci. Technol.* 35 (2021) 298–314.
- [20] V. Pandiyan, D. Cui, T. Le-Quang, P. Deshpande, K. Wasmer, S. Shevchik, situ quality monitoring in direct energy deposition process using co-axial process zone imaging and deep contrastive learning, *J. Manuf. Process.* 81 (2022) 1064–1075.
- [21] R. McCann, M.A. Obeidi, C. Hughes, E. McCarthy, D.S. Egan, R.K. Vijayaraghavan, A.M. Joshi, V.A. Garzon, D.P. Dowling, P.J. McNally, In-situ sensing, process monitoring and machine control in Laser Powder Bed Fusion: a review, *Addit. Manuf.* 45 (2021) 102058.
- [22] D. Chen, P. Wang, R. Pan, C. Zha, J. Fan, S. Kong, N. Li, J. Li, Z. Zeng, Research on in situ monitoring of selective laser melting: a state of the art review, *Int. J. Adv. Manuf. Technol.* 113 (2021) 3121–3138.
- [23] Y. AbouelNour, N. Gupta, In-situ monitoring of sub-surface and internal defects in additive manufacturing: A review, *Mater. & Des.* 222 (2022) 111063.
- [24] Y. Chen, S.J. Clark, L. Sinclair, C.L.A. Leung, S. Marussi, T. Connolley, R. C. Atwood, G.J. Baxter, M.A. Jones, I. Todd, Synchrotron X-ray imaging of directed energy deposition additive manufacturing of titanium alloy Ti-6242, *Addit. Manuf.* 41 (2021) 101969.
- [25] H. Wang, B. Gould, M. Moorehead, M. Haddad, A. Couet, S.J. Wolff, situ X-ray and thermal imaging of refractory high entropy alloying during laser directed deposition, *J. Mater. Process. Technol.* 299 (2022) 117363.
- [26] S.A. Khairallah, A.A. Martin, J.R.I. Lee, G. Guss, N.P. Calta, J.A. Hammons, M. H. Nielsen, K. Chaput, E. Schwalbach, M.N. Shah, M.G. Chapman, T.M. Willey, A. M. Rubenchik, A.T. Anderson, Y.M. Wang, M.J. Matthews, W.E. King, Controlling interdependent meso-nanosecond dynamics and defect generation in metal 3D printing, *Science* 368 (2020) 660–665.
- [27] C. Zhao, B. Shi, S. Chen, D. Du, T. Sun, B.J. Simonds, K. Fezzaa, A.D. Rollett, Laser melting modes in metal powder bed fusion additive manufacturing, *Rev. Mod. Phys.* 94 (2022) 045002.
- [28] K. Zhang, Y. Chen, S. Marussi, X. Fan, M. Fitzpatrick, S. Bhagavath, M. Majkut, B. Lukic, K. Jakata, A. Rack, Pore evolution mechanisms during directed energy deposition additive manufacturing, *Nat. Commun.* 15 (2024) 1715.
- [29] Z. Snow, E.W. Reutzel, J. Petrich, Correlating in-situ sensor data to defect locations and part quality for additively manufactured parts using machine learning, *J. Mater. Process. Technol.* 302 (2022) 117476.
- [30] J. Petrich, Z. Snow, D. Corbin, E.W. Reutzel, Multi-modal sensor fusion with machine learning for data-driven process monitoring for additive manufacturing, *Addit. Manuf.* 48 (2021) 102364.
- [31] Y. Balit, E. Charkaluk, A. Constantinescu, Digital image correlation for microstructural analysis of deformation pattern in additively manufactured 316L thin walls, *Addit. Manuf.* 31 (2020) 100862.
- [32] T. Yu, J. Zhao, Semi-coupled resolved CFD–DEM simulation of powder-based selective laser melting for additive manufacturing, *Comput. Methods Appl. Mech. Eng.* 377 (2021) 113707.
- [33] Z. Gan, G. Yu, X. He, S. Li, Numerical simulation of thermal behavior and multicomponent mass transfer in direct laser deposition of Co-base alloy on steel, *Int. J. Heat. Mass. Transf.* 104 (2017) 28–38.
- [34] Z. Nie, G. Wang, J.D. McGuffin-Cawley, B. Narayanan, S. Zhang, D. Schwam, M. Kottman, Y.K. Rong, Experimental study and modeling of H13 steel deposition using laser hot-wire additive manufacturing, *J. Mater. Process. Technol.* 235 (2016) 171–186.
- [35] F.B. Koupaei, M. Javanbakht, M. Silani, M.H. Mosallanejad, A. Saboori, Mechanics-based phase-field model for directional microstructure evolution: Multiscale finite element simulation of IN718 IN DED process, *Comput. Mater. Sci.* 261 (2026) 114342.
- [36] O. Kovalev, D. Bedenko, A. Zaitsev, Development and application of laser cladding modeling technique: From coaxial powder feeding to surface deposition and bead formation, *Appl. Math. Model.* 57 (2018) 339–359.
- [37] J.I. Arrizubieta, A. Lamikiz, F. Klocke, S. Martínez, K. Arntz, E. Ukar, Evaluation of the relevance of melt pool dynamics in Laser Material Deposition process modeling, *Int. J. Heat. Mass. Transf.* 115 (2017) 80–91.
- [38] Z. Yang, S. Wang, L. Zhu, J. Ning, B. Xin, Y. Dun, W. Yan, Manipulating molten pool dynamics during metal 3D printing by ultrasound, *Appl. Phys. Rev.* 9 (2022).

- [39] J. Shinjo, C. Panwisawas, Chemical species mixing during direct energy deposition of bimetallic systems using titanium and dissimilar refractory metals for repair and biomedical applications, *Addit. Manuf.* 51 (2022) 102654.
- [40] H. Wei, T. Mukherjee, W. Zhang, J. Zuback, G. Knapp, A. De, T. DebRoy, Mechanistic models for additive manufacturing of metallic components, *Progress. Mater. Sci.* 116 (2021) 100703.
- [41] Y. Jia, L. Jegou, E. Feulvarch, Y. Saadlaoui, V. Kaftandjian, T. Elguedj, L. Dubar, J.-M. Bergheau, An improved Arbitrary Lagrangian–Eulerian thermal-fluid model by considering powder deposition effects on melting pool during Direct Energy Deposition processes, *Addit. Manuf.* 96 (2024) 104570.
- [42] F. Wirth, K. Wegener, A physical modeling and predictive simulation of the laser cladding process, *Addit. Manuf.* 22 (2018) 307–319.
- [43] C. Soulaïne, S. Roman, A. Kovscek, H.A. Tchelepi, Pore-scale modelling of multiphase reactive flow: application to mineral dissolution with production of, *Journal of Fluid Mechanics* 855 (2018) 616–645.
- [44] M. Chung, K.-H. Lee, J. Park, Y.S. Lee, G.J. Yun, A fully computational approach for the prediction of melt pool generation of the directed energy deposition process, *J. Mech. Sci. Technol.* (2025) 1–16.
- [45] B. Chen, B. Dong, Y. Bian, S. Li, C. Tian, X. He, G. Yu, Investigation of thermal-fluid dynamics in directed energy deposition of 316L stainless steel with laser beam oscillation, *Int. J. Heat. Mass. Transf.* 249 (2025) 127267.
- [46] A. Aggarwal, V. Pandiyan, C. Leinenbach, M. Leparoux, Investigating laser beam shadowing and powder particle dynamics in directed energy deposition through high-fidelity modelling and high-speed imaging, *Addit. Manuf.* 91 (2024) 104344.
- [47] H.S. Kim, S.H. Park, Powder stream characteristics of replaceable alumina and brass nozzle tips for directed energy deposition, *Addit. Manuf.* 102 (2025) 104734.
- [48] H. Chen, Y. Sun, S. Wang, M. Yu, H. Lu, X. Lin, L. Zhu, Numerical analysis of powder-induced gas porosity in directed energy deposition: Formation, evolution, and mitigation, *Addit. Manuf.* 107 (2025) 104815.
- [49] M. Bayat, V.K. Nadimpalli, F.G. Biondani, S. Jafarzadeh, J. Thorborg, N.S. Tiedje, G. Bissacco, D.B. Pedersen, J.H. Hattel, On the role of the powder stream on the heat and fluid flow conditions during directed energy deposition of maraging steel—multiphysics modeling and experimental validation, *Addit. Manuf.* 43 (2021) 102021.
- [50] A. Aggarwal, A. Chouhan, S. Patel, D. Yadav, A. Kumar, A. Vinod, K. Prashanth, N. Gurao, Role of impinging powder particles on melt pool hydrodynamics, thermal behaviour and microstructure in laser-assisted DED process: a particle-scale DEM–CFD–CA approach, *Int. J. Heat. Mass. Transf.* 158 (2020) 119989.
- [51] M. Sattari, A. Ebrahimi, M. Luckabauer, G.-w.R. Römer, The effect of the laser beam intensity profile in laser-based directed energy deposition: A high-fidelity thermal-fluid modeling approach, *Addit. Manuf.* 86 (2024) 104227.
- [52] M. Sattari, M. Luckabauer, A. Ebrahimi, G.-w.R.B.E. Römer, Computational study of laser beam shaping in directed energy deposition using a thermal-fluid–Microstructure model, *J. Mater. Res. Technol.* 41 (2026) 7168–7194.
- [53] Z. Wang, M. Liu, Z. Luo, Z. Yan, Simultaneous modeling of powder rigid motion and molten pool evolution for powder-based additive manufacturing, *Powder Technol.* 415 (2023) 118118.
- [54] T. Yu, Y. Zhao, J. Zhao, Full-process GPU-parallelized finite volume framework for phase field modeling of brittle fracture, *Comput. Geotech.* 187 (2025) 107481.
- [55] T. Yu, J. Zhao, GPU-optimized adaptive mesh refinement for scalable two-phase resolved CFD-DEM simulations on unstructured hexahedral grids, *Comput. Phys. Commun.* (2025) 109939.
- [56] Z. Wang, M. Liu, Semi-resolved CFD–DEM for thermal particulate flows with applications to fluidized beds, *Int. J. Heat. Mass. Transf.* 159 (2020) 120150.
- [57] V.R. Voller, M. Cross, N. Markatos, An enthalpy method for convection/diffusion phase change, *Int. J. Numer. Methods Eng.* 24 (1987) 271–284.
- [58] F. Rösler, D. Brüggemann, Shell-and-tube type latent heat thermal energy storage: numerical analysis and comparison with experiments, *Heat. Mass. Transf.* 47 (2011) 1027–1033.
- [59] Z. Wang, Y. Teng, M. Liu, A semi-resolved CFD–DEM approach for particulate flows with kernel based approximation and Hilbert curve based searching strategy, *J. Comput. Phys.* 384 (2019) 151–169.
- [60] C. Panwisawas, C. Qiu, M.J. Anderson, Y. Sovani, R.P. Turner, M.M. Attallah, J. W. Brooks, H.C. Basoalto, Mesoscale modelling of selective laser melting: Thermal fluid dynamics and microstructural evolution, *Comput. Mater. Sci.* 126 (2017) 479–490.
- [61] J.L. Tan, C. Tang, C.H. Wong, Study and modeling of melt pool evolution in selective laser melting process of SS316L, *MRS Commun.* 8 (2018) 1178–1183.
- [62] A. Ebrahimi, C.R. Kleijn, I.M. Richardson, Sensitivity of numerical predictions to the permeability coefficient in simulations of melting and solidification using the enthalpy-porosity method, *Energies* 12 (2019) 4360.
- [63] T. Yu, J. Zhao, Quantifying the mechanisms of keyhole pore evolutions and the role of metal-vapor condensation in laser powder bed fusion, *Addit. Manuf.* 72 (2023) 103642.
- [64] Z. Wang, W. Yan, W.K. Liu, M. Liu, Powder-scale multi-physics modeling of multi-layer multi-track selective laser melting with sharp interface capturing method, *Comput. Mech.* 63 (2018) 649–661.
- [65] A. Di Renzo, F.P. Di Maio, Comparison of contact-force models for the simulation of collisions in DEM-based granular flow codes, *Chem. Eng. Sci.* 59 (2004) 525–541.
- [66] A.B. Stevens, C. Hrenya, Comparison of soft-sphere models to measurements of collision properties during normal impacts, *Powder Technol.* 154 (2005) 99–109.
- [67] Z. Lai, J. Zhao, S. Zhao, L. Huang, Signed distance field enhanced fully resolved CFD-DEM for simulation of granular flows involving multiphase fluids and irregularly shaped particles, *Comput. Methods Appl. Mech. Eng.* 414 (2023) 116195.
- [68] H. Zhu, Z. Zhou, R. Yang, A. Yu, Discrete particle simulation of particulate systems: theoretical developments, *Chem. Eng. Sci.* 62 (2007) 3378–3396.
- [69] R.D. Mindlin, H. Deresiewicz, Elastic spheres in contact under varying oblique forces, (1953).
- [70] Z. Wang, W. Yan, W.K. Liu, M. Liu, Powder-scale multi-physics modeling of multi-layer multi-track selective laser melting with sharp interface capturing method, *Comput. Mech.* 63 (2019) 649–661.
- [71] L. Wang, Y. Zhang, H.Y. Chia, W. Yan, Mechanism of keyhole pore formation in metal additive manufacturing, *NPJ Comput. Mater.* 8 (2022) 22.
- [72] T. Shan, J. Zhao, A coupled CFD-DEM analysis of granular flow impacting on a water reservoir, *Acta Mech.* 225 (2014) 2449–2470.
- [73] A. Aggarwal, S. Patel, A. Vinod, A. Kumar, An integrated Eulerian-Lagrangian-Eulerian investigation of coaxial gas-powder flow and intensified particle-melt interaction in directed energy deposition process, *Int. J. Therm. Sci.* 166 (2021) 106963.
- [74] R. Di Felice, The voidage function for fluid-particle interaction systems, *Int. J. Multiph. Flow* 20 (1994) 153–159.
- [75] H. Zbib, M. Ebrahimi, F. Ein-Mozaffari, A. Lohi, Comprehensive analysis of fluid-particle and particle-particle interactions in a liquid-solid fluidized bed via CFD-DEM coupling and tomography, *Powder Technol.* 340 (2018) 116–130.
- [76] M. Piton, F. Huchet, O. Le Corre, L. Le Guen, B. Cazacliu, A coupled thermal-granular model in flights rotary kiln: Industrial validation and process design, *Appl. Therm. Eng.* 75 (2015) 1011–1021.
- [77] T. Yu, J. Zhao, Quantitative simulation of selective laser melting of metals enabled by new high-fidelity multiphase, multiphysics computational tool, *Comput. Methods Appl. Mech. Eng.* 399 (2022) 115422.
- [78] A. Ebrahimi, M. Sattari, A. Babu, A. Sood, G.-W.R. Römer, M.J. Hermans, Revealing the effects of laser beam shaping on melt pool behaviour in conduction-mode laser melting, *J. Mater. Res. Technol.* 27 (2023) 3955–3967.
- [79] A. Ebrahimi, M. Sattari, S.J. Bremer, M. Luckabauer, G.-w.R. Römer, I. M. Richardson, C.R. Kleijn, M.J. Hermans, The influence of laser characteristics on internal flow behaviour in laser melting of metallic substrates, *Mater. & Des.* 214 (2022) 110385.
- [80] A. Ebrahimi, C.R. Kleijn, I.M. Richardson, Numerical study of molten metal melt pool behaviour during conduction-mode laser spot melting, *J. Phys. D Appl. Phys.* 54 (2021) 105304.
- [81] M. Bayat, A. Thanki, S. Mohanty, A. Witvrouw, S. Yang, J. Thorborg, N.S. Tiedje, J. H. Hattel, Keyhole-induced porosities in Laser-based Powder Bed Fusion (L-PBF) of Ti6Al4V: High-fidelity modelling and experimental validation, *Addit. Manuf.* 30 (2019) 100835.
- [82] L. Wang, Y. Zhang, H.Y. Chia, W. Yan, Mechanism of keyhole pore formation in metal additive manufacturing, *npj Comput. Mater.* 8 (2022) 1–11.
- [83] S. Pang, X. Chen, W. Li, X. Shao, S. Gong, Efficient multiple time scale method for modeling compressible vapor plume dynamics inside transient keyhole during fiber laser welding, *Opt. & Laser Technol.* 77 (2016) 203–214.
- [84] M. Rudman, Volume-tracking methods for interfacial flow calculations, *Int. J. Numer. Methods Fluids* 24 (1997) 671–691.
- [85] C.J. Greenshields, OpenFOAM user guide, OpenFOAM Foundation Ltd, 2015, p. 47, version 3.
- [86] S.J. Wolff, S. Webster, N.D. Parab, B. Aronson, B. Gould, A. Greco, T. Sun, In-situ observations of directed energy deposition additive manufacturing using high-speed X-ray imaging, *Jom* 73 (2021) 189–200.
- [87] C. Lv, J. Wang, H. Li, Q. Yin, W. Liu, S. Shen, Dynamics of the laser–powder interaction in the Ti6Al4V powder feeding process of laser-directed energy deposition additive manufacturing, *J. Mater. Res. Technol.* 27 (2023) 6376–6385.
- [88] M. Pilch, C. Erdman, Use of breakup time data and velocity history data to predict the maximum size of stable fragments for acceleration-induced breakup of a liquid drop, *Int. J. Multiph. Flow* 13 (1987) 741–757.
- [89] R. Rioboo, C. Tropea, M. Marengo, Outcomes from a drop impact on solid surfaces, *At. sprays* 11 (2001).
- [90] B.J. Ennis, G. Tardos, R. Pfeffer, A microlevel-based characterization of granulation phenomena, *Powder Technol.* 65 (1991) 257–272.
- [91] D.J. Harvie, M. Davidson, M. Rudman, An analysis of parasitic current generation in volume of fluid simulations, *Appl. Math. Model.* 30 (2006) 1056–1066.
- [92] R.I. Issa, Solution of the implicitly discretised fluid flow equations by operator-splitting, *J. Comput. Phys.* 62 (1986) 40–65.
- [93] M. Zhou, Z. Yang, Z. Xu, X. Song, B. Wang, Y. Zheng, Q. Zhou, G. Li, CFD-DEM modeling and analysis study of proppant transport in rough fracture, *Powder Technol.* 436 (2024) 119461.
- [94] N. Gilani, N.T. Aboulkhair, M. Simonelli, M. East, I.A. Ashcroft, R.J. Hague, From impact to solidification in drop-on-demand metal additive manufacturing using MetalJet, *Addit. Manuf.* 55 (2022) 102827.
- [95] M. Baranowski, M. Bober, A. Kudyba, N. Sobczak, The effect of surface condition on wetting of hastelloy® X by brazing filler metal of Ni-Pd-Cr-B-Si system, *J. Mater. Eng. Perform.* 28 (2019) 3950–3959.
- [96] S. He, Y. Bi, Y.-A. Shen, Z. Chen, G. Yue, C. Hu, H. Nishikawa, Contact angle analysis and intermetallic compounds formation between solders and substrates under formic acid atmosphere, *J. Adv. Join. Process.* 6 (2022) 100118.
- [97] R. Cunningham, C. Zhao, N. Parab, C. Kantzos, J. Pauza, K. Fezzaa, T. Sun, A. D. Rollett, Keyhole threshold and morphology in laser melting revealed by ultrahigh-speed x-ray imaging, *Science* 363 (2019) 849–852.