EPJ Web of Conferences **340**, 11002 (2025) https://doi.org/10.1051/epjconf/202534011002
Powders & Grains 2025

A Coupled Fluid-Granular Approach to Modelling Powder Stream in Directed Energy Deposition

Tijan Mede[1,*], *Michael* Mallon[2], *Bruno* Chareyre[3], and *Matjaž* Godec[1]

[1]Institute of Metals and Technology, Lepi pot 11, Ljubljana, Slovenia
[2]Materials and Processes Section, Structures, Mechanisms and Materials Division, Mechanical Department, ESA-ESTEC, Keplerlaan 1, 2201 AZ Noordwijk, The Netherlands
[3]University Grenoble-Alpes, CNRS, 3SR, 1270 Rue de la Piscine, Gières, France

Abstract. Metal-based Directed Energy Deposition, a key variation of additive manufacturing, has emerged as a highly promising technology for space applications. Its ability to function effectively in microgravity, along with unrestricted object size and relatively fast production times, makes it particularly attractive for this sector. However, the technology faces significant challenges, primarily concerning low dimensional precision and recurring defects linked to insufficient control and understanding of powder delivery. Recognizing the need for reliable, cost-efficient, and flexible software solutions, ESA advocates for the integration of Virtual Testing in Process-Structure-Property (PSP) modelling as a viable complement to conventional experimental methods. In response, a novel numerical framework is introduced, leveraging a full coupling of a Discrete Element solver for powder phase modelling and computational fluid dynamics for gas phase modelling to increase the simulation accuracy of powder stream dynamics.

1 Introduction

Metal-based Additive Manufacturing (AM), particularly Directed Energy Deposition (DED), is a potentially disruptive technology for the space market in demand of high-performance and low-weight structures for spacecraft [1, 2]. However, before the advantages of this technology can be fully harvested, the technology itself, as well as our understanding of it must fully mature. Advancing AM and DED would not only strengthen the European space program but also enhance the competitiveness of European manufacturing on a global scale.

The inherently stochastic nature of the powder stream in DED has long been linked to manufacturing inaccuracies and recurring defects [3–5]. Over the past two decades, various models have been developed to improve both predictive capabilities and the overall understanding of material deposition in DED.

While most conventional approaches to DED powder stream are analytical, modern state-of-the-art models are predominantly numerical. These numerical approaches primarily utilize computational fluid dynamics (CFD) to solve the two-phase flow problem, where the dispersed powder phase is modelled using an additional transport equation [6–9]. These approaches typically employ one-way coupling, meaning that while the influence of the carrier gas on the powder particles is accounted for, the reactive forces exerted by the powder particles on the gas, as well as inter-particle interactions, are disregarded. Many of the usual assumptions made in analytical modelling are not necessarily required when using advanced numerical schemes and it has been shown that some of them — such as linear particle trajectories and constant particle velocities — may not be warranted [10]. Inter-particle collisions are often omitted from numerical models of powder streams [4, 6–8, 11, 12] due to the relatively low volume fraction of powder in the carrier gas flow [8]. However, recent research suggests that particle collisions significantly influence powder stream dynamics [13, 14]. It has been proposed to expand the conventional CFD approach by detecting powder particle collisions and resolving them using the Hertz theory [13] to overcome this deficiency.

The established CFD-based approaches for modelling the powder stream in DED face the additional challenge of accurately specifying boundary conditions for the powder phase at the nozzle outlet. Some models assume a uniform velocity field for both the powder and gas phases at the outlet [6], while others include a limited section of the nozzle's inner walls in the model to simulate powder-wall interactions [4, 7, 8, 11, 12]. Consequently, the velocity distribution of powder particles at the nozzle exit is highly dependent on several factors, including the selected boundary conditions further upstream (often assumed as uniform velocity), the restitution coefficient of particle-wall collisions, and the assumed particle shape (typically spherical), which vary significantly across different studies. Some of these studies [4, 8, 11] concluded that particle velocity at the nozzle outlet is size-dependent, with larger particles losing momentum due to consecutive collisions with the inner nozzle walls, while smaller particles with sufficiently low Stokes numbers follow the carrier gas streamlines and

*e-mail: tijan.mede@imt.si

retain their velocity. However, it is important to emphasize that these findings are derived exclusively from numerical simulations and are yet to be validated experimentally.

We therefore propose a comprehensive approach to overcome the shortcomings and open challenges of the current state of the art regarding the simulative models of DED powder stream. A full coupling of Discrete Element Method (DEM) to handle the powder phase and Computational Fluid Dynamics (CFD) to handle the gas phase is proposed for improved accuracy of the blown powder dynamics. The full coupling implies that the proposed approach accounts for the drag force that the fluid exerts on the powder particles, the reactive force that the powder particles exert on the fluid as well as the inter-particle interaction during powder grain collisions. The boundary conditions for the powder phase at the nozzle outlet are experimentally evaluated to determine the powder particle velocity distribution as a function of powder grain size.

2 The powder phase

Open-source discrete element solver YADE [15] is employed to model the powder phase of the stream. Using DEM enables us to leverage state-of-the-art computational efficiency in granular dynamics and inter-particle interactions, while the open-source nature of the platform provides the flexibility required for coupling with the CFD solver. Given the high sphericity requirements for DED powders, powder particles are initially modelled as perfect spheres. However, the use of DEM allows for future modifications to incorporate particle non-sphericity if needed.

Powder particles are generated at randomly distributed positions along the nozzle outlet, with a frequency determined by the specified mass deposition rate. The radii of the generated particles are randomly assigned based on the measured particle size distribution of the simulated powder, while their initial velocities are sampled from an experimentally determined velocity distribution (see subsection Powder boundary conditions). The gravitational force acting on the particles is applied in accordance with the orientation of the simulated DED head, and Cundall's non-viscous damping is set to zero. Perfectly elastic inter-particle collisions are considered, incorporating both normal and shear contact forces [15].

Since DEM operates as an explicit numerical method, a critical time step exists beyond which the simulation becomes unstable. To ensure numerical stability, the DEM time step is set as a fraction of this critical value, preventing elastic waves from propagating beyond the minimum distance between integration points.

2.1 Powder boundary conditions

The boundary conditions for the powder phase are experimentally evaluated at the chosen DED deposition head by implementing a combination of a high-speed camera and illuminated plane (Fig. 1) to record the trajectories of the power particles exiting the DED nozzle as published in [16].

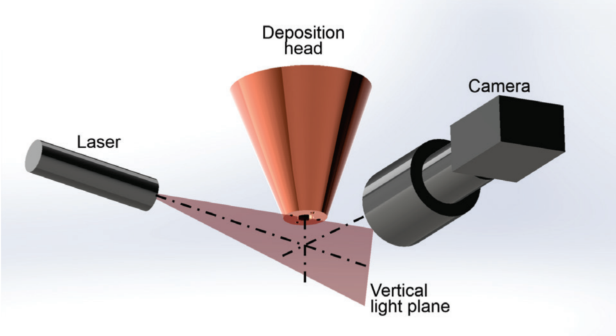

Figure 1. Experimental setup for measuring the powder boundary conditions at the DED nozzle outlet.

It was shown that using a Gaussian distribution to model the powder particle speed v and divergence angle Θ distributions produces an excellent fit with the measured distributions. The powder particle size was shown to have a strong influence on the particle velocities at the nozzle outlet and needs to be accounted for in setting up the powder boundary conditions. Powder particle initial velocities at the DED nozzle outlet are thus modelled as Gaussian distributions with particle size-dependent values for mean values and standard deviations of particle speed and divergence angle as elaborated in [16].

The powder boundary conditions do have a strong influence on the simulation results (particularly close to the nozzle) and it should be mentioned that the validity of the established boundary conditions across the entire range of deposition head types and processing conditions is yet to be validated.

3 The gas phase

Open-source CFD solver OpenFOAM is utilized to model the gas phase of the powder stream. At the highest recommended volumetric flux of carrier gas, the Reynolds number for the Argon flow through the channels of the selected DED nozzle is $Re \approx 2260 < 2300$, indicating laminar flow. However, assessing the Reynolds number of the carrier gas flow relative to the powder particles is more challenging due to the unknown velocity difference between the two phases. Since the flow velocity remains well below half the speed of sound, assuming incompressibility is reasonable [17]. Consequently, an incompressible, laminar flow model is adopted at this stage.

To solve the continuity and momentum Navier-Stokes equations, PISO pressure-velocity coupling is applied:

$$\nabla \cdot \boldsymbol{u} = 0 \tag{1}$$

$$\frac{\partial}{\partial t}(\boldsymbol{u}) + \nabla \cdot (\boldsymbol{uu}) - \nabla \cdot (\nu \nabla \boldsymbol{u}) = -\nabla p + \left(\boldsymbol{g} + \boldsymbol{f}_{hyd}\right), \tag{2}$$

where $\boldsymbol{u}$ is the fluid velocity vector, t is time, p is pressure, ν is kinematic viscosity, $\boldsymbol{g}$ is gravitational acceleration and $\boldsymbol{f}_{hyd}$ is hydrodynamic body force per unit mass (see Eq. 4).

Boundary conditions for the gas phase are set as follows (Fig. 2):

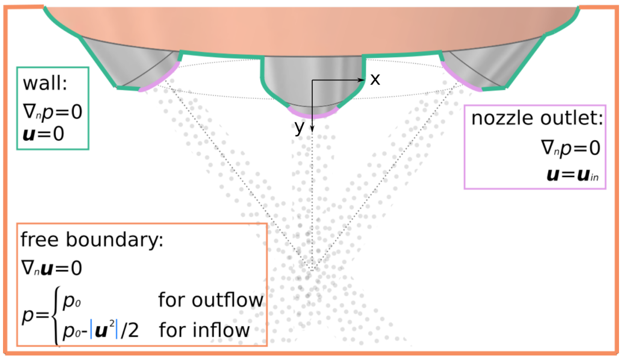

Figure 2. Fluid phase boundary conditions for the modelled system.

- for the nozzle outlet: fixed velocity ($\boldsymbol{u} = \boldsymbol{u}_{in}$) and zero pressure gradient ($\nabla_n p = 0$);
- for the free boundary: zero gradient velocity condition ($\nabla_n \boldsymbol{u} = 0$) and total pressure condition ($p = p_0$ for outflow; $p = p_0 - |\boldsymbol{u}^2|/2$ for inflow);
- for the solid walls: zero velocity ($\boldsymbol{u} = 0$) and zero pressure gradient ($\nabla_n p = 0$).

4 Coupling of the powder and gas phases

The typical mass deposition rates in DED fall in the range 10g/min < Φ_m^p < 50g/min, while the carrier gas volumetric flow rate typically varies in the range 2L/min < Φ_V^f < 8L/min. Depending on the utilized mass deposition rate and carrier gas volumetric flow rate as well as material density (typically in the range of 4000-8000 kg/m^3), the volume fraction of the powder at the outlet of the considered nozzle can be evaluated to $1.5 \cdot 10^{-4} < \alpha < 6 \cdot 10^{-3}$. Depending on the powder particle diameter, which is typically in the range 50 µm < d_p < 150 µm, and fluid velocity, Stokes number for the considered two-phase flow will result in different values of the magnitude $St \approx 10^4$. The given range of powder volume fraction and Stokes numbers suggests that the fluid forces on the powder particles and the reactive force of the particles on the fluid as well inter-particle interaction are relevant [18]. The need for four-way coupling is additionally supported by our recent study evaluating the relevance of inter-particle interactions for the considered nozzle and reporting large potions of grains being involved in inter-granular collisions [14].

Adopting the Lagrangian point-force coupling approach, the hydrodynamic force $\boldsymbol{F}_{hyd}$) on a particle is represented by a point force. Applying the Stokes drag force formulation, the letter can be expressed as:

$$\boldsymbol{F}_{hyd} = 3\pi\mu_f d_p \boldsymbol{u}_r, \quad (3)$$

where μ_f is the fluid dynamic viscosity, d_p is particle diameter and $\boldsymbol{u}_r$ is the relative velocity between the carrier gas and the particle center. The reaction force of the particle on the surrounding fluid is formulated as a body force and applied in the cell, where the particle resides. The hydrodynamic body force $\boldsymbol{f}_{hyd}$ can thus be expressed as:

$$\boldsymbol{f}_{hyd} = \frac{-\boldsymbol{F}_{hyd}}{V_c \rho_f} \quad (4)$$

where V_c is the cell volume and ρ_f is the fluid density.

The coupling interface between Yade and openFoam developed by Kunhappan et al. [19, 20] is used to perform the simulations.

5 Validation

The particle trajectories measured far from the nozzle in the high-speed camera experiment described in section 2.1 were compared against simulated results to validate the developed model on a Fraunhofer COAX 12V5 deposition head at volumetric flow rate of Argon carrier gas 5L/min. Ti-6AL-4V powder was separated into size fractions to observe the influence of particle size. An overlay of measured and simulated particle horizontal positions at a vertical distance 11mm from the nozzle are displayed in Fig. 3. Visual inspection suggests a good fit between the simulated and measured data that can be quantified with the following coefficients of determination R^2 for each particle size: R^2(0-45 µm)=0.93, R^2(45-63 µm)=0.97, R^2(63-75 µm)=0.98, R^2(75-100 µm)=0.96, R^2(100-125 µm)=0.93 R^2(125-150 µm)=0.93.

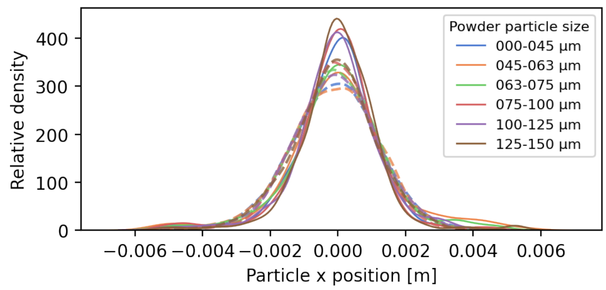

Figure 3. Simulated and experimentally measured powder particle positions at a vertical distance 11mm from the nozzle. Solid lines represent simulated distributions and dashed line represent measured distributions for individual powder particle size fractions.

6 Conclusions

The fully coupled DEM-CFD approach presented here demonstrates our strategy to address some of the pressing issues that still hinder the DED technology from achieving its full potential. Given that poor dimensional accuracy and structural defects in DED manufacturing are largely attributed to inadequate control over the powder stream, a deeper understanding of powder stream dynamics could be crucial for improving process stability. The developed computational strategy to simulating DED powder stream addresses the main gaps in existing numerical models and enhances predictive accuracy by introducing several important contributions to the field that give it edge over the rival state-of-the-art approaches: (i) The applied Lagrangian point-force coupling expands the validity of the method compared to the usually employed two-phase CFD approaches, as it remains valid even for large Stokes numbers. The latter is very relevant considering the usual range of utilised particle sizes in DED; (ii) Combining the coupled DEM-CFD numerical model with the implemented approach for measuring the powder particle velocities at the nozzle outlet ensures that the powder boundary condition and its dependency on the particle size is accurately represented; (iii) Powder particle collisions and their influence on powder stream dynamics are accounted for.

Acknowledgements

The authors acknowledge the financial support from the Slovenian Research and Innovation Agency (project No. Z2-4446 and research core funding No. P2-0132). The investigation was conducted in the scope of the European Space Agency RPA project under contract No. 4000142691/23/NL/MH/mp.

References

[1] S.M.A. Noori Rahim Abadi, P. Hagqvist, F. Sikström, I. Choquet, Cfd-based feasibility study of laser-directed energy deposition with a metal wire for on-orbit manufacturing, Frontiers in Space Technologies **3**, 880012 (2022).

[2] T.D. Ngo, A. Kashani, G. Imbalzano, K.T. Nguyen, D. Hui, Additive manufacturing (3d printing): A review of materials, methods, applications and challenges, Composites Part B: Engineering **143**, 172 (2018).

[3] S. Wen, Y. Shin, J. Murthy, P. Sojka, Modeling of coaxial powder flow for the laser direct deposition process, International Journal of Heat and Mass Transfer **52**, 5867 (2009).

[4] O. Kovalev, I. Kovaleva, I.Y. Smurov, Numerical investigation of gas-disperse jet flows created by coaxial nozzles during the laser direct material deposition, Journal of Materials Processing Technology **249**, 118 (2017).

[5] Z. Liu, H.C. Zhang, S. Peng, H. Kim, D. Du, W. Cong, Analytical modeling and experimental validation of powder stream distribution during direct energy deposition, Additive Manufacturing **30**, 100848 (2019).

[6] J. Lin, Numerical simulation of the focused powder streams in coaxial laser cladding, Journal of Materials Processing Technology **105**, 17 (2000).

[7] S. Zekovic, R. Dwivedi, R. Kovacevic, Numerical simulation and experimental investigation of gas–powder flow from radially symmetrical nozzles in laser-based direct metal deposition, International Journal of Machine Tools and Manufacture **47**, 112 (2007).

[8] P. Balu, P. Leggett, R. Kovacevic, Parametric study on a coaxial multi-material powder flow in laser-based powder deposition process, Journal of Materials Processing Technology **212**, 1598 (2012).

[9] H. Tan, C. Zhang, W. Fan, F. Zhang, X. Lin, J. Chen, W. Huang, Dynamic evolution of powder stream convergence with powder feeding durations in direct energy deposition, International Journal of Machine Tools and Manufacture **157**, 103606 (2020).

[10] A.J. Pinkerton, Advances in the modeling of laser direct metal deposition, Journal of laser applications **27**, S15001 (2015).

[11] S. Liu, Y. Zhang, R. Kovacevic, Numerical simulation and experimental study of powder flow distribution in high power direct diode laser cladding process, Lasers in Manufacturing and Materials Processing **2**, 199 (2015).

[12] C. Katinas, W. Shang, Y.C. Shin, J. Chen, Modeling particle spray and capture efficiency for direct laser deposition using a four nozzle powder injection system, Journal of Manufacturing Science and Engineering **140** (2018).

[13] Q. Chai, X. He, Y. Xing, G. Sun, Numerical study on the collision effect of particles in the gas-powder flow by coaxial nozzles for laser cladding, Optics & Laser Technology **163**, 109449 (2023).

[14] T. Mede, M. Godec, Relevance of inter-particle interaction in directed energy deposition powder stream, Powder Technology **435**, 119393 (2024).

[15] V. Šmilauer, E. Catalano, B. Chareyre, S. Dorofeenko, J. Duriez, A. Gladky, J. Kozicki, C. Modenese, L. Scholtès, L. Sibille et al., Yade reference documentation, Yade Documentation **474** (2010).

[16] T. Mede, A. Jeromen, E. Govekar, M. Mallon, M. Godec, Influence of particle size on powder velocity distribution at the nozzle outlet in directed energy deposition, Available at SSRN 5116848 (preprint).

[17] A. Otto, H. Koch, R.G. Vazquez, Multiphysical simulation of laser material processing, Physics Procedia **39**, 843 (2012).

[18] S. Elghobashi, On predicting particle-laden turbulent flows, Applied scientific research **52**, 309 (1994).

[19] D. Kunhappan, B. Harthong, B. Chareyre, G. Balarac, P.J. Dumont, Numerical modeling of high aspect ratio flexible fibers in inertial flows, Physics of Fluids **29** (2017).

[20] D. Kunhappan, Ph.D. thesis, Université Grenoble Alpes (2018)