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Validation and optimization of powder nozzle designs for DED-Machines using coupled CFD-DEM approaches

E. Uhlmann[1,2], M. Polte[1,2], S. Lezama[1], K. Bischoff[1]

[1]*Institute for Machine Tools and Factory Management IWF, Technische Universität Berlin, Germany*
[2]*Fraunhofer Institute for Production Systems and Design Technology IPK, Berlin, Germany*

lezama@iwf.tu-berlin.de

Abstract
Efficient powder delivery is critical to the performance and reliability of directed energy deposition processes in additive manufacturing. This work presents a comprehensive numerical investigation into the design and optimization of powder nozzles and distributors. To capture the complex internal geometries, polyhedral meshes with local mesh refinements were employed. Flow behavior was analyzed using Reynolds-Averaged Navier-Stokes (RANS) simulations with a k-ω shear stress transports (k-ω SST) turbulence model, extended to incorporate species transport of air and argon. This enabled local predictions of oxygen concentration in the focal zone, providing insights into oxidation risk during material processing. To assess particle dynamics under realistic conditions, CFD simulations were coupled with discrete element modeling (DEM) using ANSYS Fluent and ANSYS Rocky. The coupled approach allowed for the evaluation of key jet characteristics of the powder nozzles including powder focus diameter, focus distance, and divergence angle, with similarity to design targets. Further simulations of the powder distributors revealed powder accumulation zones within the distributor, linked to recirculating flows and low-velocity regions. These findings guided geometry modifications to improve flow uniformity, which were validated through reduced CFD-only simulations, significantly lowering computational demand. In parallel, physical prototypes of powder channels were fabricated using wire EDM to study the influence of surface roughness on particle transport, using a 70 % CNCS and 30 % NbC powder blend. Predictive tuning of nozzle geometries based on target output parameters could be achieved by fine-tuned Regression Models, supporting the development of automated design tools for powder delivery systems.

Directed energy deposition (DED), powder nozzle design, computational fluid dynamics (CFD), particle flow simulation

1. Introduction

Directed Energy Deposition (DED) is a laser-based additive manufacturing processes widely used for producing complex geometries, repairing high-value components, and applying wear- and corrosion resistant coatings. Achieving high process quality and efficiency depends critically on precise powder delivery through well-designed nozzle systems. Powder distribution at the focal plane directly affects deposition accuracy, material utilization and oxidation risk during processing [1].

Computational Fluid Dynamics (CFD) modeling has proven to be essential for understanding gas-particle interactions in DED nozzles. Accurate turbulence modeling is particularly important to resolve internal carrier gas flow and jet formation. Ostolaza et al. [2] demonstrated that conventional k-ε turbulence models tend to underestimate centerline velocity and perform poorly in transitional and free-jet flows typical of powder nozzles. By contrast, the k-ω Shear Stress Transport (SST) model provided better predictions of nozzle outflow behavior and improved agreement with experimental measurements of powder stream focus diameter and focal distance [2].

Beyond internal flow, interactions between carrier gas, shield gas, and ambient atmosphere can entrain surrounding air, disturb protective gas coverage, and reduce powder convergence at the melt pool. CFD simulations have shown that higher carrier gas flow rates improve stream convergence by increasing particle velocity v_P, but shield gas flows can spread the powder stream and reduce central concentration. Optimizing these parameters through simulation enables nozzle designs that achieve higher powder supply efficiency and reduced material waste, as shown in previous nozzle geometry designs with measured efficiency improvements [1].

Furthermore, the inner surface roughness of powder channels has been shown to strongly influence powder propagation behavior. Channels with lower surface roughness reduce the divergence angle of the powder stream by up to 61 % and increase particle velocities by over 28 %, enabling tighter focuses and greater working distances at lower carrier gas flow rates. These effects are critical to achieve consistent, efficient powder delivery with lower gas consumption and improved process robustness [3].

In this work a comprehensive numerical investigation aimed at the design and optimization of powder nozzles and distributors to improve powder delivery efficiency, focus quality and process robustness in DED applications is presented.

2. Methodology

The powder nozzle and distributor geometries were modeled to capture the complex internal flow paths. Polyhedral meshes with local refinements were generated to resolve critical regions of the nozzle throat and powder distributor, with mesh sensitivity studies guiding the final element sizes. Flow simulations were performed using Reynolds-Averaged Navier–Stokes (RANS) equations with a k-ω Shear Stress Transport (SST) turbulence model to accurately represent confined and free jet transitions. A species transport model for air and argon (Ar) was implemented to predict local oxygen concentrations c_{O2} in the focal zone, allowing assessment of oxidation risk during material processing. Powder particle dynamics were evaluated using a coupled CFD–DEM approach, linking ANSYS Fluent 2024 R1 with ANSYS Rocky 2024 R1, from ANSYS, Inc., USA. The discrete phase model tracked individual particle trajectories and interactions with the nozzle walls. Key performance indicators were defined as the powder focus diameter d_{PF}, focus distance l_{PF}, and divergence angle β of the powder jet. For the powder distributor, both CFD-only and coupled CFD–DEM simulations were performed to identify the role of recirculating flows and low-velocity regions in causing uneven powder distribution among channels. The results were used to assess when reduced CFD-only simulations could serve as a rapid evaluation tool with lower computational demands. Additionally, simplified nozzle geometries, as shown in Figure 1, were simulated to derive regression models linking key geometric parameters, including channel diameter d_{PK}, channel length l_{PK}, channel offset s_{PK}, and powder injection angle α, to process output metrics (d_{PF}, l_{PF}, particle velocity v_P). These models provide the basis for automated design optimization. Physical prototypes powder channels, with channel diameter d_{PK} =1.5 mm, were fabricated via wire EDM (WEDM) to investigate the effect of inner surface roughness on particle dispersion using a 70 % CNCS / 30 % NbC powder blend. The experimental results are correlated with numerical predictions to validate the impact of roughness on divergence angle and particle velocity [3].

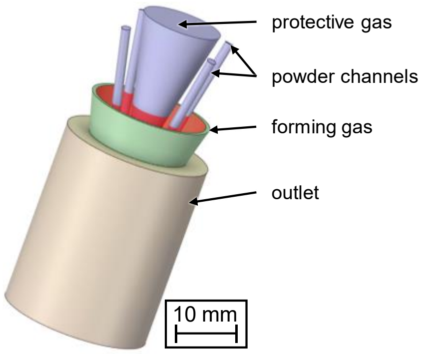

Fig. 1. Simplified nozzle geometry for coupled CFD-DEM simulations

3. Results and discussion

The simulated powder jet characteristics for the nozzle designs showed similarity to the defined target values, Table 1.

Table 1 Comparison of target values T and numerical simulation values S; 1) focus diameter d_{PF}; 2) focus length l_{PF}; 3) divergence angle β

Indicator	Nozzle Type 1		Nozzle Type 2		Nozzle Type 3	
	T [mm]	S [mm]	T [mm]	S [mm]	T [mm]	S [mm]
1	< 2.20	1.74	< 2.00	1.36	< 2.20	1.32
2	13.00	12.50	14.00	13.50	14.00	14.00
3	< 4.00	3.50	< 4.00	3.60	< 4.00	2.96

Species transport simulations revealed oxygen concentration distributions c_{O2} within the focal zone, Figure 2. Furthermore, the ability to identify oxidation-prone regions and supporting design modifications for processing reactive alloys is demonstrated. Analysis of the powder distributor highlighted the presence of recirculation zones and low-velocity pockets that led to uneven powder feeding into the four outlet channels. CFD–DEM results confirmed particle accumulation in these areas. Comparison with CFD-only runs showed that key flow features could be captured without particle tracking, reducing computational time significantly and enabling rapid iteration of distributor designs. Geometry modifications derived from these insights were implemented, and new distributor prototypes are currently under evaluation.

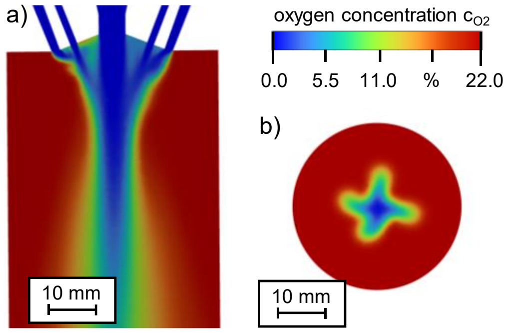

Fig. 2. Oxygen concentration c_{O2} a) nozzle cross section b) focus plane

The investigation confirmed the relationship between inner channel surface roughness Ra and powder propagation behavior. Higher surface roughness Ra values led to increased divergence angles and reduced particle velocities, in agreement with experimental findings from high-speed imaging. The wire EDM-fabricated channels provided reference data to validate this effect for the 70 % CNCS / 30 % NbC powder blend, showing a reduction of divergence angle β of over 50 % when the surface roughness Ra decreased from Ra = 2.1 µm to Ra = 0.3 µm [3].

The regression models derived from the simplified geometry simulations reflect the link between nozzle design parameters and process outcomes. This enables predictive tuning of nozzle designs based on target focal spot characteristics, forming the foundation for an automated nozzle design tool.

4. Conclusion

A coupled CFD–DEM framework was developed to optimize powder nozzles and distributors for DED. The k-ω SST turbulence model with species transport enabled accurate prediction of powder jet characteristics and oxygen concentration c_{O2} in the focal zone. Simulation results confirmed a close match between designed and computed focus diameter d_{PF}, distance l_{PF}, and divergence angle β. Analysis of powder distributors identified recirculation zones as the main cause of uneven flow, and CFD-only models were shown to provide a fast approximation for geometry evaluation. Experimental studies on powder channel roughness validated the simulations, demonstrating that smoother channels significantly reduce divergence angles β and increase particle velocities v_P.

The results highlight the effectiveness of simulation-driven optimization in improving powder delivery efficiency and process reliability in DED.

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