Gas flow study for development of a novel shielding gas nozzle for directed energy deposition processes using computational fluid dynamic simulations

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Abstract. Directed energy deposition (DED) enables the additive manufacturing of several materials such as molybdenum alloys that are very difficult to process by conventional methods. Some of these materials are highly reactive to gases in ambient atmosphere such as oxygen and nitrogen. Oxidation during additive manufacturing significantly influences the mechanical properties of a part. In some cases, the shielding gas coverage of standard powder nozzles is not sufficient, and oxidation still takes place. A functional prototype of a compound multi flow path annular nozzle was developed using computational fluid dynamic simulations. Simulations were performed using multi-component miscible gas model. Prototypes were manufactured for several design iterations to test their functionality in cold flow conditions. In the end, an Inconel based prototype was built, using laser powder bed fusion. The volume of shielding gas cover over the substrate improved with the proposed design and the radial extent of 80 ppm oxygen concentration increased from 8 mm to 25 mm. Finally, Mo-Si-B alloy was deposited on a 1000 °C pre-heated substrate without significant oxidation or cracks.

1. Introduction
Additive manufacturing (AM) plays an important role in digitalization of manufacturing industries. Laser metal deposition (LMD) is a DED technique in which material powder is melted by laser beam and deposited layer by layer. The technique of LMD provides the aspects of flexibility of manufacturing in terms of materials and shapes [1]. One of the major limitations with this process is maintaining the quality of the build. Oxidation is a major factor determining the final mechanical properties of the build which occurs at different temperatures for different materials. Oxidation can be restricted by reducing the concentration of oxygen in the zone of metal deposition by displacing the oxygen with inert gases [2]. A popularly used method is to fill a physical chamber with inert gases and perform metal deposition inside the chamber [3]. This is economically and temporally a demanding process. Besides the use of a physical chamber, a localized inert atmosphere of shielding gases can be used. This local atmosphere can be achieved by using nozzle systems to effectively deliver the inert gas and shield the metal from...
oxidation. Mostly nozzles are designed to deliver material powder coaxially with laser beam. Material powder is transported with a carrier gas which is also inert in nature [3]. A lot of research has been performed on effects of shielding gas on metal deposition techniques and the parameters that effect the shielding phenomena such as gas flow rate, and the type of gas [4, 5]. For the LMD setup used in this work, a commercially available coaxial nozzle from Precitec is used. However, such commercial nozzles showed limitations in shielding the process zone. Especially, strong oxidation occurred when processing materials with high affinity for oxygen such as molybdenum alloys. Therefore, in this work, the influence of shielding gas flows from a conventional nozzle and a specially designed additional nozzle was investigated using computational fluid dynamic (CFD) simulations.

2. Material and Methods

2.1. Material
The material used in this study is an alloy of molybdenum, silicon and boron. Mo-Si-B is an alloy which can be used for parts operating in ultra-high temperature zones due to its melting temperature over 2000°C [6]. The substrate used in this study was a titanium-zirconium-molybdenum cylinder with a radius of 20 mm. The powder used for deposition was a Mo-Si-B alloy with the chemical composition listed in Table 1.

Table 1. Chemical composition of Mo-Si-B used in this study.

| Component | Molybdenum | Silicon | Boron |
|-----------|------------|---------|-------|
| Atomic %  | 76         | 16.5    | 7.5   |

2.2. Experimental set-up
The experimental set-up with the additional shielding gas nozzle is shown in Figure 1. The equipment, which is shown in Figure 1, is a specifically developed test setup from Siemens. This test setup consists of a motion control SINUMERIK 840D, a TRUMPF laser TRUDisk 8002, a medium-frequency generator MFG70 for preheating, and a vibration powder feeder from MediCoat for the powder supply. The SINUMERIK 840D controls the laser, the processing system, and the vibration powder feeder. The process chamber consists of a Precitec laser processing head, the developed additional shielding gas nozzle, a three-axis motion system, and an inductor with a pyrometer for control of the preheating temperature. The track height of the deposited material was monitored by a distance sensor of Precitec, which measures the distance of the LMD nozzle to the melting zone to guarantee a uniform distance across all layers in the z-direction. The diameter of the laser beam was 800 µm and the focal length was 300 mm. The feeding fibre core diameter was 400 µm and the collimation was 150 mm. Argon has been used as a shielding gas as well as carrier gas for the powder. In the experiments, a cube with an edge length of 10 mm was built. The process strategy was based on an outer frame which was filled by a meander strategy. The process parameters used for the experiments are shown in Table 2.

Table 2. Process parameters used for the experiments.

| Parameter | Total powder mass flow | Travel speed | Laser power | Laser wavelength | Hatching space | Track height | Preheating |
|-----------|------------------------|--------------|-------------|------------------|----------------|--------------|------------|
| Value     | 1.60 g/min             | 0.4 m/min    | 240 W       | 1030 nm          | 0.4 mm         | 0.4 mm       | 1000°C     |
2.3. Experimental measurement method
The main metric measured in this study is the concentration of oxygen. Experimentally, a residual oxygen meter ORBmax from Orbitalum was used which gives the concentration in terms of parts per million (ppm). The device uses optical sensor technology and works on the principle of fluorescence extinction. It works with an accuracy of 10% of the value displayed. The concentration of oxygen was measured at the centre of the process zone, where the laser and powder focus are located, by drawing the gas through a small hole in a plate located below the nozzle.

2.4. Computational simulation method
In this study, the finite volume method approach was used to simulate the flow of multiple miscible gases and predict their concentrations. The computational domain is divided into smaller units called as control volumes. Several partial differential equations are discretised for these control volumes and solved for the required quantities in those equations. The main concept behind this approach is to conserve the mass, momentum and energy of a given flow in each control volume and the whole computational domain [7].

\[
\frac{\partial}{\partial t} \int_V \rho Y_i dV + \oint_A \left[ \rho Y_i (\mathbf{v} + \mathbf{M}_i) \right] \cdot d\mathbf{a} = \oint_A \left[ J_i + \frac{\mu_t}{\sigma_t} \nabla Y_i \right] \cdot d\mathbf{a} + \int_S S Y_i dV \tag{1}
\]

In addition to flow conservation equations of mass, momentum and energy, one more equation known as species transport equation from Siemens Star-CCM+ was solved to determine the concentrations of the miscible gases in the domain as shown in equation (1). The parameters used are: \( V \) = volume, \( Y \) = mass fraction, \( i \) = component index, \( a \) = area vector, \( M \) = migration term in electric field, \( J \) = laminar (molecular) diffusive flux, \( \sigma_t \) = turbulent Schmidt number, \( S \) = source term, and \( \mu_t \) = turbulent viscosity. Concentration of the required species was measured in terms of ppm which is derived from mole fraction computed from mass fraction in equation (1).

2.5. Simulation setup
The digital models for the nozzle were designed using Siemens NX. These models were later used for development of the additional nozzle. Geometry preparations, meshing and CFD simulations for this study were performed in Siemens Star-CCM+. Investigations of the designs were performed by reducing the computational domain to 2D axis-symmetrical models with a polygonal mesh [8]. Detailed analysis of the final design was performed by simulating 3D models with polyhedral mesh. Two layers of prismatic cells were generated along the wall to capture the wall effects inside the nozzle [9, 10]. Mesh was refined till the extent where an iso-line representing 1 ppm concentration of air was not affected by
changing the mesh size further. A base mesh size of 1 mm was applied on the whole computational domain with a minimum cell size of 0.1 mm to maintain at least 4 cells between two adjacent walls.

Simulations were performed in steady state where the flow is assumed to be not changing with time [7]. The fluids in this study were argon and air. Multi-component gas model was used for the simulations. It considers the fluids as miscible and non-reacting. Ideal gas model was chosen to perform the simulations as there were no huge density changes due to Mach number of the flow. Temperatures were not considered, and iso-thermal model was applied to the simulations. Realizable two-layer all y+ K-Epsilon turbulence model was used to model the flow in the viscous regime. Segregated solver from Siemens Star-CCM+ was used to perform the simulations.

2.6. Conventional nozzle
The existing conventional nozzle is a coaxial compound nozzle. Figure 2 shows the different flow paths of the nozzles. The main gas flow is used as shielding gas of the process and the side gas flow is used as shielding gas and as carrier gas of the metal powder which is necessary for an accurate powder focus. The baseline boundary conditions used for the CFD simulations are shown in Table 3. ‘Outlet’ is the outer boundary of the computational domain around the nozzle. For the ‘Main Flow’ and ‘Side Flow’, the flow rates which are mentioned in terms of liters per minute (lpm) are converted into velocities based on the cross-sectional areas of the nozzle inlets.

| Boundary   | Type            | Value |
|------------|-----------------|-------|
| Main Flow  | Velocity Inlet  | 18 lpm|
| Side Flow  | Velocity Inlet  | 12 lpm|
| Outlet     | Pressure Outlet | 0 Pa  |

2.7. Additional nozzle
Taking into consideration the analysis of flow behavior from the conventional nozzles, an additional nozzle was designed which could shield the entire substrate region. This nozzle was designed with two separate flow paths which could be mounted upon the conventional nozzle system. Figure 3 depicts the cross section of the computational domain with existing nozzle flow paths ‘A’ and ‘B’, additional nozzle flow paths ‘C’ and ‘D’, substrate, and workbench.
A porous region was incorporated into the outer flow path ‘D’. The additional nozzle boundary conditions used in the CFD simulation are shown in Table 4. Nitrogen was used through the flow path ‘D’ as it was abundantly available at higher pressures. The porous region was designed as a lattice structure which is feasible to manufacture in laser powder bed fusion (LPBF). The structural and porous properties of the lattice structure are shown in Table 5. The lattice structure was converted into a porous region to be used in Siemens Star-CCM+ for flow simulations. The porous properties were calculated by performing simulations on the lattice structure and using Darcy-Forchheimer formulation [11, 12].

Table 4. Boundary conditions used to simulate the additional nozzle.

| Boundary       | Type         | Fluid  | Value |
|----------------|--------------|--------|-------|
| A (Main Flow)  | Velocity Inlet | Argon  | 14 lpm |
| B (Side Flow)  | Velocity Inlet | Argon  | 6 lpm  |
| C              | Velocity Inlet | Argon  | 14 lpm |
| D              | Velocity Inlet | Nitrogen | 60 lpm |

Table 5. Physical properties and calculated porous coefficients of the lattice structure.

| Lattice Type       | Pore edge (mm) | Porosity | Porous inertial coefficient (kg/m$^3$) | Porous viscous coefficient (kg/m$^3$-sec) |
|--------------------|----------------|----------|----------------------------------------|------------------------------------------|
| Tri-diametral      | 0.7            | 54%      | 12,763                                  | 5,828                                    |

3. Results

3.1. Conventional nozzle

To understand the flow behaviour with the conventional nozzle, simulations were performed and compared with recordings from experimental tests. Figure 4 shows the air concentration in a 2D computational domain for the base flow conditions of the conventional shielding gas nozzle. It can be imagined as an axis-symmetric slice of the nozzle.

Figure 4. Scalar plot of concentration of air from simulation of conventional nozzle.
It shows the different boundaries used in the simulation. ‘R’ depicts the radial distance from the axis of the nozzle to the extent of 80 ppm of air on the substrate level which was found to be 8 mm. Another analysis was performed to check if the used gas flow rates from Table 3 were suitable and if the spread of shielding gas was sensitive to the flow rates. It was observed that radial distance ‘R’ depends directly on the main flow and inversely on the side flow. Figure 5 shows the plot of results from the simulation. The case of ‘Base flow rate’ uses the conditions mentioned in Table 3. Similar trend was observed from experimental recordings.

3.2. Additional shielding gas nozzle

Figure 6 shows the scalar plot of concentration of air for different nozzle-to-work distances when the additional shielding gas nozzle is implemented. It was observed that the entire substrate region of 20 mm radius was covered with shielding gas by maintaining the concentration of oxygen below 80 ppm, also for a nozzle-to-work distance of 21 mm. Therefore, the shielding is sufficient to build parts with a height of at least 10 mm.

![Figure 6](image)

**Figure 6.** Scalar plot of concentration of air from simulation of the additional shielding gas nozzle at a) a nozzle height of 11 mm and b) a nozzle height of 21 mm.

![Figure 7](image)

**Figure 7.** a) Vertical section and b) horizontal section of the 3D model of the additional shielding gas nozzle c) manufactured nozzle by laser powder bed fusion from Inconel 625
The solid part of this nozzle design was built keeping the flow paths similar to that of the simulated design. Figure 7 (a) and Figure 7 (b) shows the two cross-sections of the 3D model of the additional nozzle and Figure 7 (c) shows the manufactured nozzle. Two coolant paths were introduced into the nozzle as it operates at high temperatures around 1000°C. Nozzle and its features were designed to be additively manufactured from Inconel 625 by LPBF.

The manufactured metallic additional nozzle was mounted on the conventional nozzle. Initially, oxygen concentrations were measured in cold conditions without metal deposition process. Recordings were taken for multiple nozzle-to-work distances. It was observed that in cold flow conditions, the spread of shielding gas with the additional nozzle, covered the whole region of substrate below 80 ppm of oxygen as predicted from simulations. Figure 8 shows the experimental recordings of oxygen concentration for the additional nozzle-to-work distance of 11 mm.

The labels in the image depict the concentration of oxygen in terms of ppm at respective coordinates relative to the centre of the process zone (0, 0). It was observed that the ppm values increased rapidly, approximately at the radial distance of outer flow path ‘D’. During actual processing, the substrate was heated up to 1000°C with an induction ring and material was deposited.

Figure 9 (a) shows the part built of Mo-Si-B by using the additional nozzle. A cube with side length of 10 mm was successfully deposited on the substrate. Figure 9 (b) shows the cross-section of the deposited cube. In the process without additional shielding gas nozzle, the substrate showed a high level of oxidation and decolouration after preheating to 1000°C and it was not possible to proceed processing with these oxidation effects. No cracks were observed inside the cube when additional nozzle was used to provide shielding gas as seen from Figure 9 (b).
4. Discussion

4.1. Conventional nozzle

The conventional compound nozzles are used to deliver shielding gas, and material powder onto the substrate. The cover of shielding gas provided by this nozzle system was insufficient to deposit Mo-Si-B and even cover the entire substrate region with less than 80 ppm of oxygen. The reason for insufficient coverage of shielding gas even after increasing flow rate can be attributed to the nature of jet flow and jet mixing. Figure 10 shows some of the important parts of a jet emerging out of a round nozzle.

In our case, the outer nozzle which consists of flow path ‘B’ from Figure 3, has a very small outlet diameter as it is designed to deliver material powder. Therefore, it has a smaller potential core which does not support in shielding the process zone. The potential core of the inner nozzle with flow path ‘A’ from Figure 3 provides the overall shielding effect.

In addition to diameter ‘d’ of the nozzle exit as shown in Figure 10, the jet mixing also depends on the velocity of the flow. It was found in studies that a higher flow rate results in higher Reynolds number (Re) of the flow which enhances the mixing of the jet with ambient atmosphere [15, 16]. The dependence of velocity profiles of a jet flow on Reynolds number can be seen from Figure 11. The velocity profiles are plotted for a H/D ratio of 10 [14]. Velocity profiles depict how quickly the jet disperses into the ambient atmosphere. The centre-line velocity decays very rapidly at higher Re number. It can be inferred therefore that the jet mixing would increase with increase in flow rate. The reason for reduction of ‘R’ with increase in flow rate as shown in Figure 5 can be attributed to the dependence of jet mixing on Reynolds number as shown in Figure 11.

![Figure 9](image_url)

**Figure 9.** a) Deposited structure when using the additional shielding gas nozzle. b) Cross-section of the printed Mo-Si-B cube.

![Figure 10](image_url)

**Figure 10.** Depiction of potential core and parts of jet as based on [13].
4.2. Additional Nozzle

4.2.1. Potential core of annular nozzle. The issue of having a limited potential core with the conventional nozzle was addressed by the additional nozzle. Flow from additional nozzle acted as an annular shielding wall around the processing zone thereby separating the inert gases delivered by conventional nozzle from the ambient atmosphere as can be seen from Figure 12. A wider annular flow path was designed for flow path ‘D’ as can be seen from Figure 3 to have a wider non-mixing zone.

![Figure 12. Depiction of mixing zones a) w/o additional nozzle and b) with additional nozzle.](image)

4.2.2. Lattice structures. Lattice structures reduced the effective flow volume inside the nozzle and because of its porous nature, aided in distributing the flow inside the nozzle. A larger annular radius of additional nozzle demanded a very high flow rate of shielding gas. The shielding gas was delivered through pipes which have a very small internal diameter compared to the nozzle. Because of its higher flow rate and sudden change in flow areas, from pipes to nozzle, the shielding gas did not fill the nozzle completely leaving some pockets of ambient air. Therefore, lattice structures were designed to diffuse the shielding gas inside the nozzle and completely displace ambient air from the nozzle. In addition to distributing the flow, porous nature of lattice structures helped in reducing the turbulence of the flow.

5. Conclusions

To reduce the jet mixing with ambient atmosphere during powder DED and enable stable processing without oxidation effects, the gas flow should be maintained in the laminar regime of the flow. It was shown that the shielding gas flow can be stabilized by additionally applied gas flows, while the super positioning of the potential core of the jets was found to have the main impact on the gas mixing. Increasing annular radius of additional nozzle demands an increase in the flow rate of shielding gas to completely fill the nozzle without any pockets of ambient air inside the nozzle. Properly designed lattice structures improved the flow distribution inside the nozzle and provided a better flow uniformity at nozzle exit. CFD simulations were used to understand the flow behaviour of the gases. Lattice structures were modelled as porous region for the simulations. Fibre based prototypes of the additional nozzles were built to validate the simulations and provide an agile feedback in the design loops. An Inconel
based prototype was built using LPBF for the final design of the additional nozzle. The newly developed additional nozzle system was able to prevent extensive oxidation during DED of Mo-Si-B deposition. A cube of 10 mm edge length was successfully deposited by using the additional nozzle. No cracks were observed from a cross-section of the cube.

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