

Validation of computational fluid dynamics method through experimental investigation of the plasma spraying process

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Abstract. Numerical modelling has emerged as a powerful predictive tool to enhance plasma sprayed coatings quality and process efficiency. In the present work, a comprehensive Computational Fluid Dynamics model of a gas heating inside a direct current arc plasma torch, is developed, using the simulation software Ansys Fluent. It is therefore sought to test its accuracy and limitations by comparing its predictions to actual data generated in the South African Nuclear Energy Corporation plasma spraying laboratory. In this regards, titanium powder of respective size distributions, 0-63 µm, and 63-75 µm, is sprayed onto a metal piece work. The transport medium is an argon-nitrogen plasma jet, generated from a direct current torch running under an induced power of 12.8 – 13.1 kW. The spraying distance and powder carrier gas flow rate are varied throughout the experiment, from 75 to 85 mm, and 3.9 to 5.8 kg/h, respectively. Comparison of laboratory and simulation-based results were mostly in agreement, in terms of the plasma jet shape, the effect of power increase on the torch exit temperature, the effects of particle size distribution, and carrier gas variation on particle melting and trajectory.

1 Introduction

Throughout recent years, Plasma Spraying has been one of the most widely used spraying techniques in view of its versatility and cost-efficient characteristics [1]. Direct Current (DC) Plasma Spraying relies on the ability of an electric arc, generated inside a DC plasma torch, to ionize the gas jet stream and produce a plasma jet. The partial ionization of the plasma jet is achieved through the passage of the electric current from the cathode to the anode. Following the generated plasma jet increase in temperature and velocity, coating particles are injected into the jet and subsequently melted and accelerated towards the desired substrate, leaving a uniform thin coating of substance on the substrate [2]. However, one of the main challenges encountered by this technology has been attaining the highest reproducibility of high-level properties coatings. Numerical modelling of the plasma spray process is required

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for optimizing spray parameters and improving our understanding of complex heat, momentum, and mass transport phenomena involved [3]. This paper focuses on validating through experimentation, a well-developed comprehensive numerical model to simulate plasma jet formation inside a direct current (DC) plasma torch, and subsequent heat flow and mass exchange between injected particles and ionized gas.

2 Methodology

2.1 Mathematical Modelling

2.1.1 Plasma flow

It is assumed that the generated plasma jet flows through and out of the torch under the following conditions: it behaves as an ideal gas being in local thermodynamic equilibrium, subjected to turbulent flow, in such a way that it is optically thin, incompressible, and can be considered as a Newtonian continuous fluid at one temperature [4-6]. Furthermore, gravitational effect and viscous dissipation are considered negligible, while the transport coefficients and thermodynamic properties of argon-nitrogen plasma are functions of the local temperature [7]. In addition, electrical and magnetic fields are ignored as the electrical arc is substituted by a cylindrical plasma source term inside the torch nozzle.

Based on the aforementioned assumptions, the transport equations, consisting of the continuity (1), momentum (2), energy (3), equation of state (4), and turbulent (5, 6) equations are expressed as follows:

$$\nabla \cdot (\rho \vec{V}) = 0 \quad (1)$$

$$\nabla \cdot (\rho \vec{V} \vec{V}) = -\nabla P + \nabla \cdot \bar{\tau} + \vec{F} \quad (2)$$

$$\nabla \cdot [(e + P) \vec{V}] = \nabla \cdot (\lambda \nabla T) + \emptyset d + Qj - Qr \quad (3)$$

$$P = \rho R T \quad (4)$$

$$\nabla \cdot (\rho \vec{V} k) = \nabla \cdot (\Gamma x \nabla k) + G - \rho \varepsilon \quad (5)$$

$$\nabla \cdot (\rho \vec{V} \varepsilon) = \nabla \cdot (\Gamma \varepsilon \nabla \varepsilon) + C\varepsilon 1 G \frac{\varepsilon}{k} - C\varepsilon r \rho \frac{\varepsilon^2}{k} \quad (6)$$

Here, \vec{V} , P , $\bar{\tau}$, e , λ , T , \emptyset_d , Qj , Qr , ρ , R , k , Γ_x , G , ε , Γ_ε , $C_{\varepsilon 1}$, and $C_{\varepsilon r}$ are, respectively, velocity vector, fluid pressure, viscous stress tensor, internal energy, thermal conductivity, fluid temperature, dissipation loss, joule heating, radiation loss, density, gas constant, turbulent kinetic energy, transport coefficient for kinetic energy, generation rate of kinetic energy, dissipation rate of kinetic energy, transport coefficient for dissipation rate, and constant.

2.1.2 Particle injection and in-flight behaviour

In order to model a coating particle's journey through the generated plasma jet, starting with their injection, there is a need to establish a set of assumptions that would at the same time simplify the complex particle-plasma interaction, while retaining good predictive capabilities. Thus, the following assumptions are formulated [3, 8]:

- Titanium is considered as the powder material
- Titanium powder is injected internally, just before the torch exit
- Particles are spherical
- Particle-particle interactions are neglected
- Particle velocity derives from the carrier gas
- Particles are accelerated by the drag force of the plasma gas

- Particle internal temperature is uniform
- The carrier gas flow rate is not time-dependent
- The injector walls are smooth and straight
- Momentum and energy transfer are the basic interaction mechanisms between particles and the plasma stream
- Radiative heat transfer is considered

Following the above stated assumptions, it is possible to determine the velocity and trajectory of powder particles through momentum mechanisms. For particle trajectory, the inertia, drag force and gravity are expressed as:

$$\frac{d\vec{U_p}}{dt} = F_D (\vec{u} - \vec{U_p}) + \frac{\bar{g}(\rho_p - \rho)}{\rho_p} + \vec{F} \quad (7)$$

$$F_D = \frac{18 \mu}{\rho_p d^2 p} \frac{Cd Re}{24} \quad (8)$$

Where \vec{u} , $\vec{U_p}$, μ , ρ , ρ_p , d_p , Re , \vec{F} , F_D ($\vec{u} - \vec{U_p}$) are, respectively, fluid velocity, particle velocity, fluid viscosity, fluid density, particle density, particle diameter, Reynolds number, any source term per unit particle mass, and drag force per unit particle mass.

On the other hand, the heat transfer from the plasma flow to the particle is given by:

$$m_p C_p = h A_p C_p (T_\infty - T_p) + \epsilon_p A_p \sigma (T_w^4 - T_p^4) + Q_{\text{Melting}} + Q_{\text{Evaporation}} \quad (9)$$

Where m_p , C_p , T_p , A_p , T_∞ , T_w , ϵ_p , σ , Q_{Melting} , and $Q_{\text{Evaporation}}$ are, respectively, mass of particle, specific heat, particle temperature, particle surface area, plasma temperature, wall temperature, particle emissivity, Stefan-Boltzmann constant, latent heat, and evaporation heat [2].

2.2 Numerical modelling

Based on measurements of the non-transferred laboratory DC plasma torch, a three-dimensional geometry was developed in Ansys Fluent, to model the fluid domain whereby plasma generation and particle-plasma interaction would take place. The computational domain catered for inlets boundaries of the incoming argon-nitrogen gas mixture, and titanium particles, as shown in Figure 1. Moreover, the anode wall and cathode are included, and a volume inside the anode nozzle is set as the energy source term.

The computational body was subsequently meshed, generating up to 1.48 million cells, followed by the setting of appropriate boundary conditions. These include the imposition of a convective heat transfer coefficient of $10^5 \text{ W/m}^2\text{-K}$ on the inner side of the anode, while the cathode surface was set at 3500 K. In addition, to simulate particle-plasma interaction, the Discrete Phase Model (DPM) provided in Ansys Fluent, was introduced, allowing the treatment of two separate phases, namely, the continuous (fluid) and the discrete phase [3]. As opposed to the continuous phase, which is treated as a continuum by solving the Navier-Stokes equations, the discrete phase on the other hand is solved by tracking a large number of particles through the calculated flow field.

Finally, with Ansys Fluent being a finite volume-based solver, governing equations as previously formulated, were successively solved for each cell through the SIMPLE algorithm incorporated withing the CFD software.

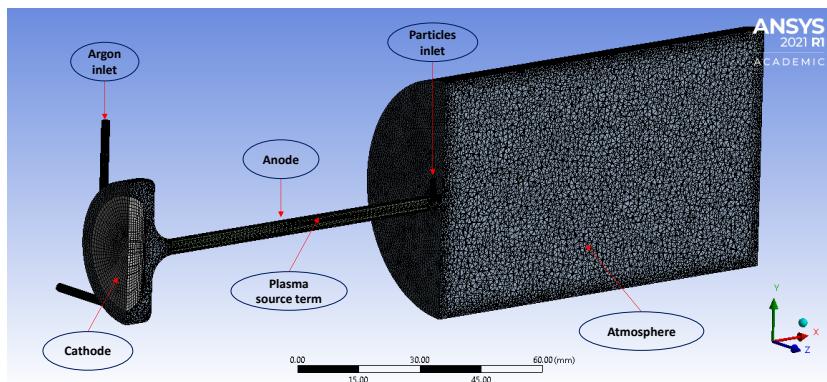


Fig. 1. Plasma torch computational domain

2.3 Experimental procedure

Titanium powders of respective size ranges 0 – 63 µm and 63 – 75 µm, were prepared. The was then collected inside a container, from which it could be injected into the metalling spraying box, precisely at the torch exit. The non-transferred DC plasma torch was subsequently assembled, and its exit was inserted into the metallic spraying box, in such a way that it was perpendicularly aligned to the powder injection port.

Argon and nitrogen gas were allowed to flow to the plasma torch, through a prepared inlet pipe, at respective flow rates of 1.88 kg/h and 4.39 k/g. In addition, cooling water was allowed to flow by the cathode and anode. After ensuring the aforementioned steps were completed, the power source was switched on, and the voltage and current were set respectively within the following ranges: 75 – 79 V, and 166 – 169 A. The resulting electric current ignited the incoming gas mixture, creating a hot plasma stream, that transported, melted, and deposited the injected titanium powder onto the metal work piece inside the spraying box.

Parameters variation included power input (12.1 – 13.5 kW), spraying distance (75 – 85 mm), particle size (0 – 63 µm to 63 – 75 µm), and carrier gas flow (3.9 – 5.8 kg/h). Energy balance around the plasma torch, and microscope analysis, respectively allowed the determination of the exit plasma stream temperature and the analysis of the coating structure after spraying. The experiment was repeated three times to ensure the validity of observations made and conclusions reached.

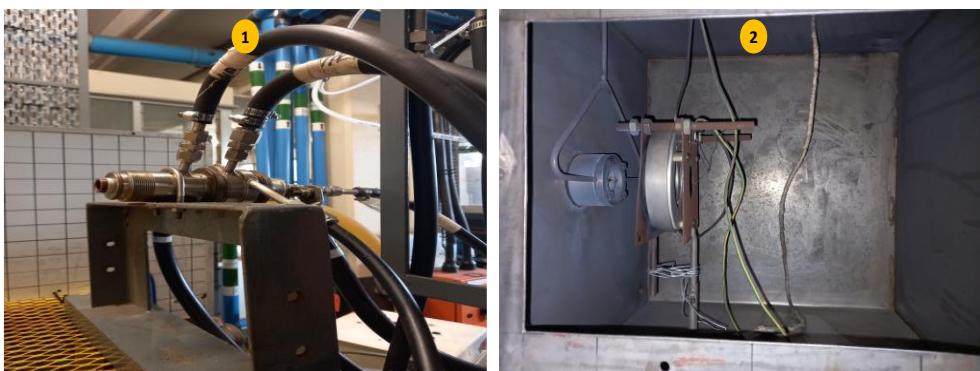


Fig. 2. Plasma torch (1) and metallic spraying box (2)

3 Results and discussion

3.1 Plasma jet

Figure 3 shows two different plasma jets illustrations. On the left, the temperature distribution of the generated plasma jet from simulation results, and on the right, an image of the plasma flow coming out of the torch, from laboratory experiments. The aim being to validate the created model, it is necessary to compare both images.

A careful observation allows to note similarities in terms of the shape of the plasma jet. Furthermore, it appears that in both cases the intensity of the plasma fades in a similar way, as the emitted light becomes weaker the further away it is from the torch exit. This is an indication of a gradual decrease in temperature, from the torch exit to the substrate.

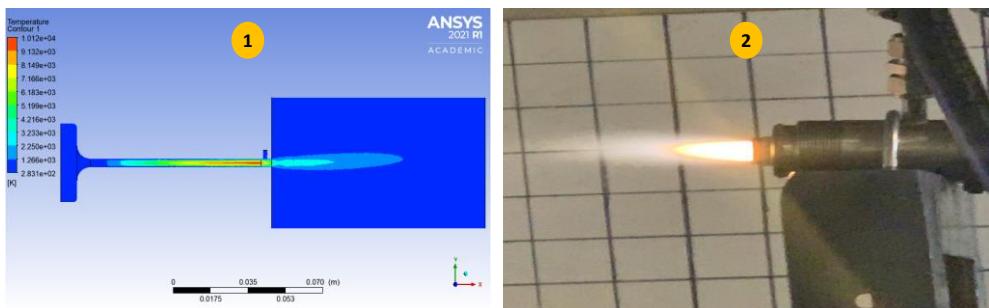


Fig. 3. Comparison between simulation-based (1) and laboratory-generated (2) plasma jets

3.2 Particles trajectory through plasma stream

Figure 4(1) shows the generated particles trajectory through the plasma stream, from simulation results. It is a difficult proposition to optically observe the behaviour of injected particles through the plasma flow, during a practical experiment, as the phenomenon occurs within seconds, and the emitted light from the plasma blinds accurate sight.

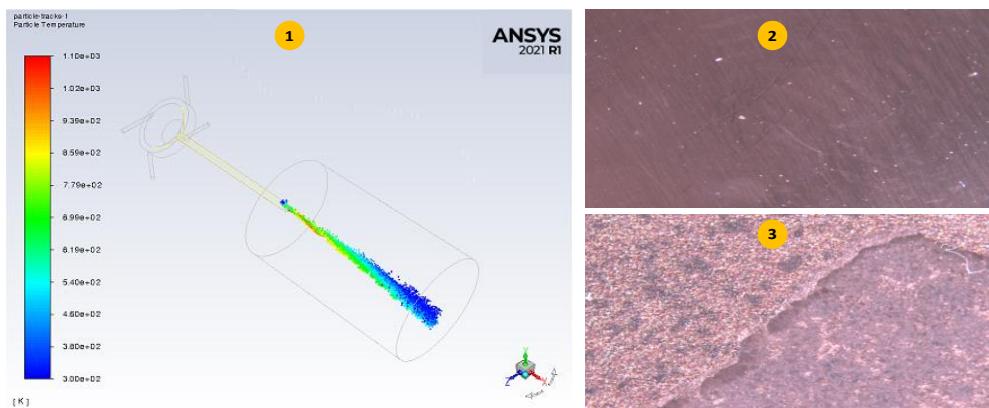


Fig. 4. Particles trajectory through plasma stream

However, observation of the coated material before and after spraying can give indications on the level of accuracy of the model predictions, as a consistent and steady stream of particles in terms of temperature and velocity would yield a quality coating, as concluded by Safaei Ardakani [2], whose numerical and experimental studies on the arc fluctuation in a

DC Plasma Torch showed that fluctuating temperature and velocity profiles at the torch outlet create different conditions for particles, which would prevent their uniform acceleration, heating, and melting, thus reducing the coating quality.

Figures 4(2) and 4(3) show respectively, images from a high precision microscope, of the coated material before, and after spraying. Observation of the two figures shows that a coating is formed on the metal piece work as predicted by the model.

3.3 Effect of power input variation on torch exit temperature

In general, an increase in the supplied electrical current, i.e., input power, accelerates the gas ionization leading to an increase of the injected particles velocity and temperature [8, 9]. In this study, the computational fluid dynamics model predicted a sharp and almost linear increase of the plasma torch exit temperature as shown in Figure 5.

To experimentally validate the above statement, the current and voltage were respectively increased from 166 to 169 A, and 75 to 79 V, thus translating to a power increase from 12.5 to 13.1 kW. The corresponding exit torch temperature for every power value was determined by calculating the enthalpy, using the total gas mass flow and the remaining power after heat transfer to the anode and cathode for cooling.

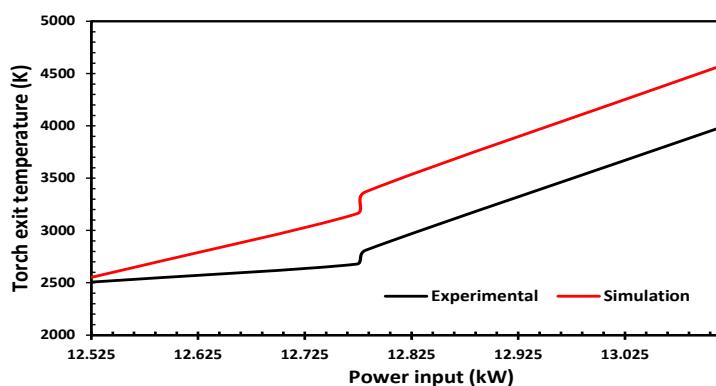


Fig. 5. Torch exit temperature as a function of power

The resulting computational and experimental temperature trends were similar as they both linearly increased with increasing input power, though their values at specific variable points differed. This discrepancy originates from the fact that exit torch temperatures were not experimentally determined using a high precision measuring device, but instead through calculations that only considered heat transfer from the plasma to the cooling water through convection, neglecting any radiation. Furthermore, this method assumed a homogeneous exit torch radial temperature distribution, while the computational model predicted different radial temperature layers, with the core being hotter than subsequent layers. However, the overall percentage error being below 20%, and the two temperature trends having similar tendencies, this experimental method can be deemed to have successfully validated simulation-based predictions.

3.4 Effect of carrier gas flow rate variation on particles velocity and temperature profiles

The momentum of powder particles, being imparted by the carrier gas to penetrate into the plasma jet and be entrained by it [10], it was sought to determine how varying the carrier gas flow would affect the resulting particles velocity and temperature profiles.

The computational fluid dynamics method predicted that increasing the carrier gas flow from 3.9 to 5.8 kg/h, while keeping all other conditions constant, would cause the injected particles to develop higher velocities as they travel towards the substrate, as shown in Figure 6(a). This would result in particles having a shorter residence time inside the plasma jet, and consequently having lower heat transferred to them from the plasma gas, leading to lower particle temperatures, and possible incomplete melting as shown in Figure 6(b).

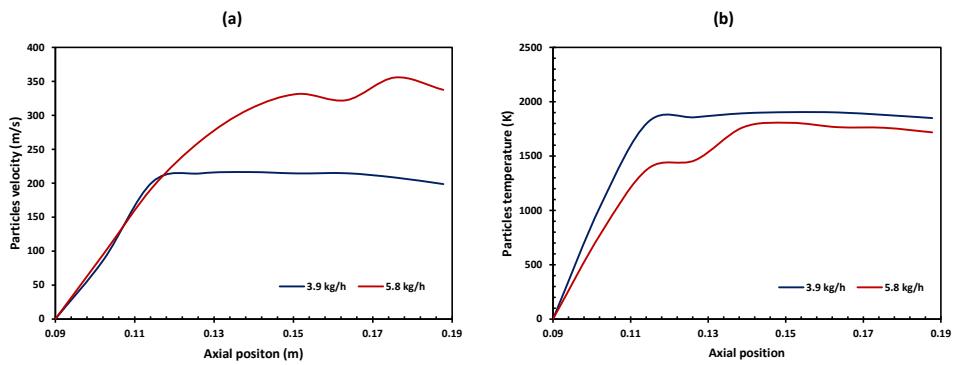


Fig. 6. Effect of carrier gas flow rate variation on (a) particle velocity (b) particle temperature

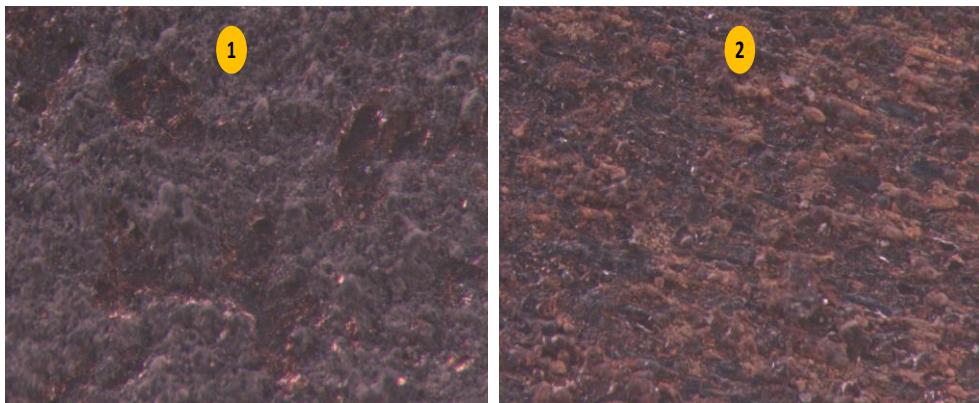


Fig. 7. Microscope images of coated material at carrier gas flow rates of (1) 3.9 kg/h and (2) 5.8 kg/h

To experimentally validate the above prediction, the most accurate route would be the use of emission spectroscopy, enthalpy probes or the HiWatch CS system to get real time data on in-flight particles surface temperature, velocity, and position. However, the aforementioned methods being quite expensive, an alternative route would be an optical observation of the coated material for every variable change, as it could give valuable information in terms of particles velocity and degree of melting at the point of impact. In this regard, microscope images of the coated material are shown in Figure 7, for respective carrier gas flows. It is

observed that for the lower carrier gas flow of 3.9 kg/h, the coated surface appears smoother than the latter, which has a rough surface with brownish inclusions, indicating a lower impact temperature, due to an increase of the carrier gas flow to 5.8 kg/h, as predicted by the computational fluid dynamics model.

3.5 Effect of particle size distribution on particles velocity and temperature profiles

To determine the effect of particles size distribution on particles velocity and temperature profiles, two particles size distribution ranges, respectively 0 – 63 μm and 63 – 75 μm , were selected and their resulting velocity and temperature profiles from the torch exit to the substrate were computed in Ansys Fluent. As shown in Figure 8(a), the computational method predicted that particles with a higher size have lower velocities in their journey towards the substrate. This is due to the fact that the level to which a particle can accelerate is heavily dependent on its weight. Lighter particles reach higher velocities as they oppose negligible opposition to the plasma jet movement, compared to heavier particles [3, 8]. Correspondingly, lighter particles reach higher temperatures, as they receive heat from the plasma quicker due to their low weight.

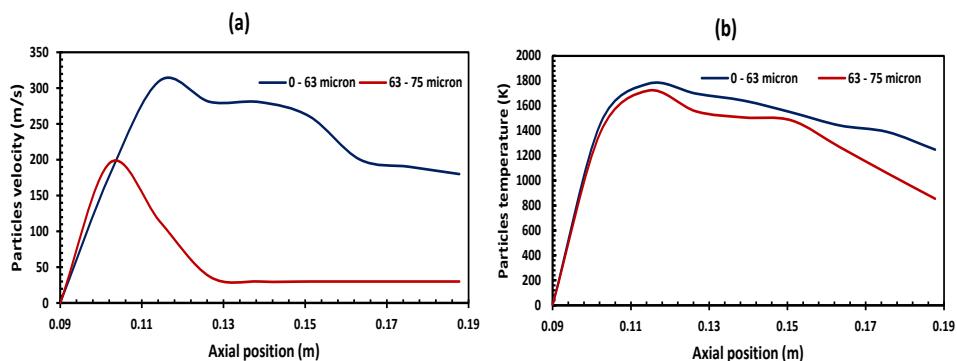


Fig. 8. Effect of particle size distribution on (a) particle velocity (b) particle temperature

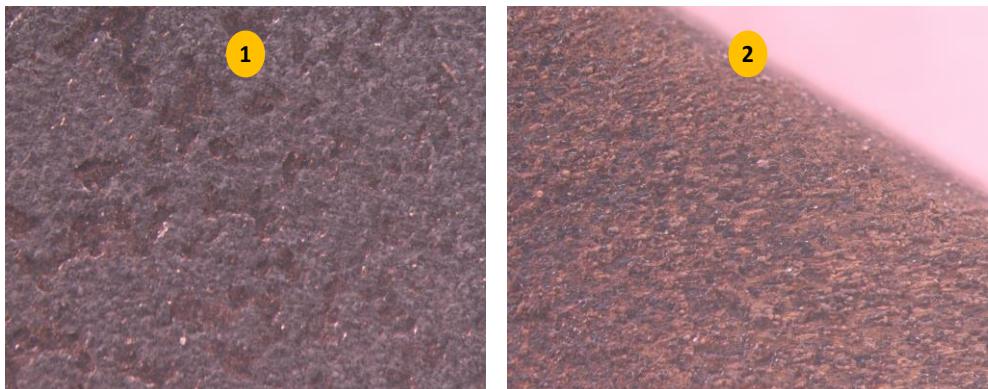


Fig. 9. Microscope images of coated material at particles size distribution ranges of (1) 0 – 63 μm and (2) 63 – 75 μm

To experimentally validate the above computational predictions, as for the carrier gas effect case study, coated materials for experimental runs with respective particle size distribution

ranges of $0 - 63 \mu\text{m}$ and $63 - 75 \mu\text{m}$, were observed at a high precision microscope as shown in Figure 9. It resulted in the lower size particles a more even surface compared to the higher size particles, for which it can be observed a large number of brownish and not completely melted spots, confirming the predictions made by the computational fluid dynamics model.

4 Conclusion

This research work aimed at undertaking an experimental laboratory investigation to validate a plasma spray computational fluid dynamics model, built in Ansys Fluent. It appears that laboratory and simulation based results were mostly in agreement, as it resulted that (1) a power input increase favors an increase in plasma jet temperature; (2) particles size distribution plays a key role in particles heating and trajectory history; (3) there is a gradual decrease of temperature and velocity from the torch exit to the spraying point; and (4) the carrier gas flow rate must be carefully calibrated to facilitate the transport of injected particles by the incoming plasma stream, and cater for enough residence time for proper heating and melting of particles.

5 Acknowledgments

The authors would like to acknowledge the Department of Science and Innovation (DSI), through the Advanced Materials Initiative (AMI) and the South African Nuclear Energy Corporation (Necsa) for financial support ; the Research and Innovation Division at Necsa for the use of their facilities; and Necsa personnel: Mr M.M. Makhofane and Mr P.C. Smith for assistance (plasma experiments). The Center for High Performance Computing (CHPC) at CSIR Campus, Rosebank, Cape Town, South Africa, is acknowledged for providing computational resources that have contributed to the research results reported within this paper.

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