Numerical Coupling of the Particulate Phase to the Plasma Phase in Modeling of Multi-Arc Plasma Spraying

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Abstract. Inherent to Euler-Lagrange formulation, which can be used in order to describe the particle behavior in plasma spraying, particle in-flight characteristics are determined by calculating the impulse, heat and mass transfer between the plasma jet and individual powder particles. Based on the assumption that the influence of the particulate phase on the fluid phase is insignificant, impulse, heat and mass transfer from particles to the plasma jet can be neglected using the so-called numerical approach of "one-way coupling". On the other hand, so-called "two-way coupling" considers the two-sided transfer between both phases. The former is a common simplification used in the literature to describe the plasma-particle interaction in thermal spraying. This study focuses on the significance of this simplification on the calculated results and shows that the use of this simplification leads to significant errors in calculated plasma and particle in-flight characteristics in three-cathode plasma spraying process.

1. Introduction

Coating formation in plasma spraying takes place as a result of continuous deposition of the molten and semi-molten particles on to the workpiece surface. Particle in-flight characteristics, i.e. their velocities, temperatures, diameters and melting grades, determine the coating quality and deposition efficiency. Particle in-flight characteristics themselves are determined by the impulse, heat and mass transfer between the plasma jet and the powder particles.

Several numerical models have been developed in the last decades, focusing on the plasma jet-particle interaction in the single-arc plasma spraying process. These have all contributed to an in-depth understanding of the impulse and heat transfer onto the particles during their residence in the plasma jet. Several models with different abstraction levels have been developed and great progress has been achieved in this field [1-12].

All previous works which have dealt with particle-plasma interaction in plasma spraying have in common that the authors have employed different model simplifications to explain certain aspects, mostly dealing with so-called non-transferred conventional single-arc plasma generators. A comprehensive numerical research focusing on plasma-particle interaction in the case of new generation multi-arc systems has not been conducted yet. One of the major assumptions employed in numerical works done so far is that the influence of particles on plasma jet characteristics is negligible in plasma spraying. The aim of this study is therefore to investigate this effect and identify the validity of the above-mentioned assumption. Meanwhile, this study focusses on multi-arc plasma spraying of ceramic feedstock materials.

2. State of Art

Heat and mass transfer between the plasma jet and the injected powder particles can principally be calculated using the Euler-Euler approach or the Euler-Lagrange approach. In both cases, a distinction is made between the continuous (plasma gas) and the dispersed phase (particles). The Euler-Euler approach treats both phases as a continuum in which they can penetrate and influence each other. The Euler-Lagrange approach on the other hand describes only the plasma gas as a continuum, whereas the particles are described as a discrete phase. By calculating the momentum transfer acting on the particles, the trajectories can be predicted and calculated. Similarly, by calculating the heat transfer, the temperatures of the particles can be determined. Due to its simplicity and robustness, the Euler-Lagrange approach dominates the literature dealing with the modelling of plasma-particle interaction in thermal spraying.

The momentum transfer in a plasma jet is influenced by several forces including virtual drag force, virtual mass force, pressure gradient force, basset force, turbulent dispersion force and external forces such as electric, magnetic and gravitational forces [13]. Although the influences of different types of forces might vary in significance depending on the powder and feed stock material characteristics as well as on injection and process conditions, all forces except the viscous drag play a secondary role in the momentum transfer between plasma jet and powder particles. This might be attributed to the fact that the densities of the feedstock materials in plasma spraying are significantly higher than that of the plasma gas. Please refer to [13] for further discussion regarding the significance of different force terms on the momentum transfer.

In the broadest sense, heat transfer between plasma jet and particles takes place as a result of convection, radiation and mass transfer. Convective heat transfer is generally considered to be more significant compared to other heat transfer mechanisms. Investigations show that although the heat transfer due to radiation gains importance with increasing spraying distance, the overall heat transfer due to convection is usually two orders of magnitude higher in comparison to radiation [14].

Euler-Lagrange approach requires the determination of the drag and heat transfer coefficients between the species of the flow for the calculation of momentum transfer due to drag forces and for the calculation of heat transfer due to convection. The equations used to determine these coefficients in case of ordinary flow conditions need to be further modified in order to make them suitable for the flow conditions in thermal spraying. In the literature, different correction factors considering the particularities of thermal plasma jets have been proposed for this purpose. For example, steep temperature gradients across the boundary layers surrounding the single particles cause the temperature dependent transport and thermodynamic properties of the plasma gas to change drastically across this layer. Determining the drag and heat transfer coefficients based on the properties of the plasma gas outside this layer would lead to erroneous results. Therefore, adjustments by means of a correction factors have been employed in the literature in order to take this effect into consideration [15-20]. Similarly, the Knudsen effect and basset history forces have been treated using correction factors [13, 17, 20-23], when required.

Mass transfer between particles and the plasma jet can occur as a result of evaporation of molten droplets or due to the chemical reaction between the particle phase and plasma gas constituents, i.e. due to oxidation. The physical evaporation of the feedstock material can be modeled using simple heat transfer models by controlling the vaporization rate with heat flux divided by latent heat of vaporization [24, 25]. On the other hand, vaporization due to volatile species requires more complicated models. Only in a few works, the numerical modeling of this phenomenon in thermal spraying is reported [12, 15, 26]. In their respective work, Wan et al. give a good overview of these activities [27].

Previous works which have dealt with the particle-plasma interaction in thermal spraying [1-12] have one thing in common: the authors have employed different model simplifications to explain certain aspects. A discussion about these simplifications, their underlying assumptions or their significance goes beyond the scope of this paper. This paper focusses on the common assumption that the influence of particles on plasma jet characteristics is negligible in plasma spraying and deals with the influence of corresponding model simplification to the results. None of the above-mentioned works has dealt with the significance of numerical back-coupling of powder particles, which allows the particles to influence the fluid phase via source terms of heat, momentum and mass on the results.

3. Mathematical Model and Boundary Conditions

Plasma exits the plasma generator at the nozzle outlet at high temperature and velocity. The set of equations which are used for modeling the plasma jet outside the plasma torch corresponds to the set of equations used for plasma generator simulations with the exception of the equations describing electromagnetic phenomena. For an overview, please refer to [28, 29]. The Euler-Lagrange approach is used in this work in order to study the particle behavior in plasma jet. The calculation domain involves the region downstream of the torch outlet. The boundary conditions and the calculation domain used in this study are presented in Figure 1.
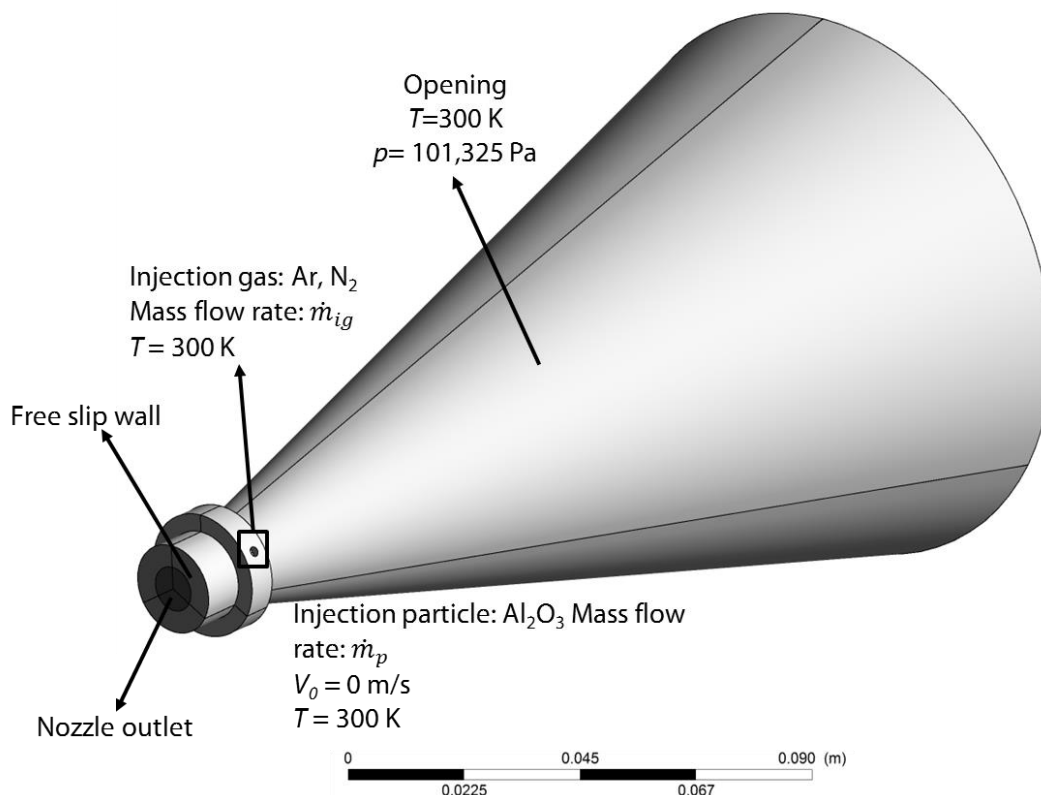

Opening
$T = 300$ K
$p = 101,325$ Pa

Injection gas: Ar, N_2
Mass flow rate: $\dot{m}_{ig}$
$T = 300$ K

Free slip wall

Injection particle: Al_2O_3 Mass flow rate: $\dot{m}_p$
$V_0 = 0$ m/s
$T = 300$ K

Nozzle outlet

| 0 | 0.045 | 0.090 (m) |
| 0.0225 | 0.067 | |

Figure 1.   Boundary conditions of the particle-plasma interaction model

The boundary conditions at the nozzle outlet are imported from a-priori conducted plasma generator simulations. Details of the model which is used to describe the physical processes in a three-cathode plasma generator have already been published in [30]. The developed model dealing with the flow characteristics of the plasma jet is introduced in [31]. The opening boundary condition at the outer surface of the calculation domain represents the flow behavior in the infinity of the air atmosphere. Moreover, an inlet boundary condition has been defined, over which powder particles are

injected in the calculation domain with defined mass flow rates, velocities and size distributions. The material data used in the simulations are listed in Table 1. The specific heat capacity of the feedstock material is defined as temperature and physical state-dependent using NASA polynomials. Values of latent heat of fusion and boiling are calculated using the enthalpies of the corresponding states at melting and boiling temperatures. The enthalpy values are calculated once again using NASA polynomials [32]. Although Al_2O_3 exhibits higher thermal conductivities of about $\kappa = 37$ W/mK at room temperature, this value decreases rapidly down to $\kappa = 5\text{-}6$ W/mK at temperatures higher than $T = 1,200$ K [33, 34]. In this work, for the sake of simplicity, a constant value of thermal conductivity, which is corresponding to the value of it at higher temperatures, is used.

Table 1: Material data used in the plasma-particle interaction simulations

Al_2O_3	Solid state	Liquid phase	Gas phase
Density [g/cm^3]	3.95	2.7	0.001[a]
Thermal conductivity [W/mK]	6	6	-
Specific heat capacity [J/kgK]	~600-900[b]	~1950[b]	~1200[b]
Latent heat of fusion (kJ/kg)		1060	
Latent heat of boiling (kJ/kg)		8885	
Melting point [K]		2327	
Boiling point [K]		3250	

[a] assumed value
[b] defined temperature dependent in the models

The particle motion in plasma spraying as a result of the drag force (F_D) is described according to equation (1). The value of the drag coefficient (C_D) in this equation depends on the particle's Reynolds number (Re_p) and forms the basis of the momentum transfer calculations. The correlation between the drag coefficient and the particle's Reynolds number employed in this study corresponds to the correlation proposed by Vardelle et al. in [20], as depicted in equation (2). Re_p itself is a function of density (ρ_g) and dynamic viscosity (μ_g) of plasma gas, particle diameter (d_p) and slip velocity between particle and plasma gas (s) as expressed in equation (3). In this study, the varying properties of the plasma gas across the boundary layer of the particle are accounted for using a simple averaging conducted over five temperature points lying between plasma gas (T_g) and particle temperature (T_p)

$$F_D = m_p \frac{dv_p}{dt} = \frac{1}{2} C_D A_p \rho_g |v_p - v_g| (v_g - v_p) \tag{1}$$

$$C_D = \begin{cases} \dfrac{24}{Re_p}, & Re_p \leq 0.2 \\[2mm] \dfrac{24}{Re_p}\left(1 + 0.1 Re_p^{0.99}\right), & 0.2 < Re_p < 2 \\[2mm] \dfrac{24}{Re_p}\left(1 + 0.11 Re_p^{0.81}\right), & 2 < Re_p < 21 \\[2mm] \dfrac{24}{Re_p}\left(1 + 0.189 Re_p^{0.62}\right), & 21 < Re_p \leq 500 \\[2mm] 0.44, & 500 < Re_p \end{cases} \tag{2}$$

$$Re_p = \frac{\rho_g s \, d_p}{\mu_g} \tag{3}$$

The convective heat transfer (Q_c) between plasma jet and particles is described according to equation (4). In this equation, h stands for the heat transfer coefficient. It is often convenient to express the heat transfer coefficient in terms of a dimensionless Nusselt number (Nu_p) as it is shown in equation (5). For a particle moving in plasma jet, Nu_p is a function of the particle's Reynolds number (Re_p) and gas Prandtl number (Pr_g). The correlation between Nu_p, Re_p and Pr_g employed in this study corresponds to the correlation proposed by Hughmark in [35], as depicted in equation (6). Pr_g is a function of specific heat capacity (Cp_g), dynamic viscosity (μ_g) and thermal conductivity (κ_g) of plasma gas according to the relationship expressed in equation (7). Analog to the situation for the drag coefficient, the varying plasma gas properties across the boundary layer of the particle are accounted for using a simple averaging.

$$Q_c = hA_i\bigl(T_g - T_p\bigr) \tag{4}$$

$$h = \frac{\kappa_g Nu_p}{d_p} \tag{5}$$

$$Nu_p = \begin{cases} 2 + 0.60 Re_p^{0.50} Pr_g^{0.33}, & 0 \le Re_p < 776.06 \text{ and } 0 \le Pr_g < 250 \\ 2 + 0.27 Re_p^{0.62} Pr_g^{0.33}, & 776.06 \le Re_p \text{ and } 0 \le Pr_g < 250 \end{cases} \tag{6}$$

$$Pr_g = \frac{Cp_g \mu_g}{\kappa_g} \tag{7}$$

In order to calculate the phase change without resolving the temperature distribution within the particle, a simple mathematical formulation is proposed and used. The melting rate ($\dot{m}_{s\to l}$) in kg/s is correlated with the heat transfer rate between plasma gas and particle (1st term) as well as with the averaged conductive heat transfer rate within the particle (2nd term), according to the equation (8):

$$\dot{m}_{s\to l} = \begin{cases} \dfrac{\pi \kappa_g Nu_p d_p (T_g - T_p)}{L_f} + \dfrac{\pi \kappa_p d_p (T_p - T_{m,p})}{L_f}, & T_{m,p} < T_p \\ 0, & T_{m,p} > T_p \end{cases} \tag{8}$$

Equation (8) describes mathematically that the rate of the phase change is determined by the heat transfer rate divided by the latent heat of fusion (L_f). Phase change does not take place at particle temperatures below the melting point of the feedstock material ($T_{m,p}$). By coupling the energy sink term ($\dot{m}_{s\to l}\cdot L_f$) into the energy equations of the gas flow, the implementation of the mathematical formulation into the model is closed. Please note that, inherent to the characteristics of the Lagrangian formulation, the particle temperatures (T_p) in equation (8) correspond to "lumped" particle temperatures. This means that no distinction between the surface temperatures and temperatures within the particle is made. Moreover, the developed model accounts for the re-solidification of the particles, too. A similar approach underlying equation (8) has been employed for this purpose. The energy released due to re-solidification has in this case been coupled into the energy equations of plasma gas flow as an energy source term.

Mass transfer between particles and plasma jet due to physical evaporation is described according to equation (9). In this equation, $\dot{m}_{l \to g}$ stands for the rate of evaporation. $T_{b,p}$ and L_b are boiling point and latent heat of boiling for the feedstock material. The mathematical formulation is coupled with the energy equations through the energy sink term ($\dot{m}_{l \to g} \cdot L_b$). The resulting particle vapor is transmitted to the Euler phase via the mass source term ($\dot{m}_{l \to g}$). Other mass transfer mechanisms, for example due to emergence of some persistent or volatile reaction products, are not taken into consideration.

$$\dot{m}_{l \to g} = \begin{cases} \dfrac{\pi \kappa_g Nu_p d_p (T_g - T_p)}{L_b}, & T_{b,p} < T_p \\ 0, & T_{b,p} > T_p \end{cases} \tag{9}$$

4. Results and Discussion

In case of the so-called numerical approach of "one-way coupling", only the influence of the fluid phase on the particulate phase is considered and the influence of the particulate phase on the fluid phase is neglected. On the other hand, "two-way coupling" allows the particles to influence the fluid phase via source terms of heat, momentum and mass. The former is a common simplification used in literature and is justified with the rate of particle injection being too low in plasma spraying to influence the plasma jet [12].

The model introduced in chapter 3 describes the behavior of ceramic powder particles in a plasma jet generated by means of a three-cathode plasma generator. Accounting the typical size distribution and material properties of the feedstock material Al_2O_3, some of the momentum and heat transfer mechanisms have been neglected. The model developed in this study takes almost all relevant effects into account, including melting, re-solidification and physical evaporation of the particles. Merely evaporation as a result of decomposition of the ceramic feedstock materials below the boiling point is not taken into consideration, the relevance of which is not investigated and clarified completely yet. Therefore, the model offers a good basis in order to analyze the differences resulting from "one-way" and "two-way coupling" approaches.

In Figure 2, the results of the simulations conducted with "one-way" and "two-way coupling" are illustrated. The comparison is conducted for a particle mass flow rate of $\dot{m}_p = 24$ g/min per injector. This is a typical rate for ceramic feedstock materials employed in thermal spraying. Powder which has an assumed normal particle size distribution with a mean value of $\mu = 30$ μm and a standard deviation of $\sigma = 10$ μm is injected from the same position in both cases. All the other parameters are kept constant.
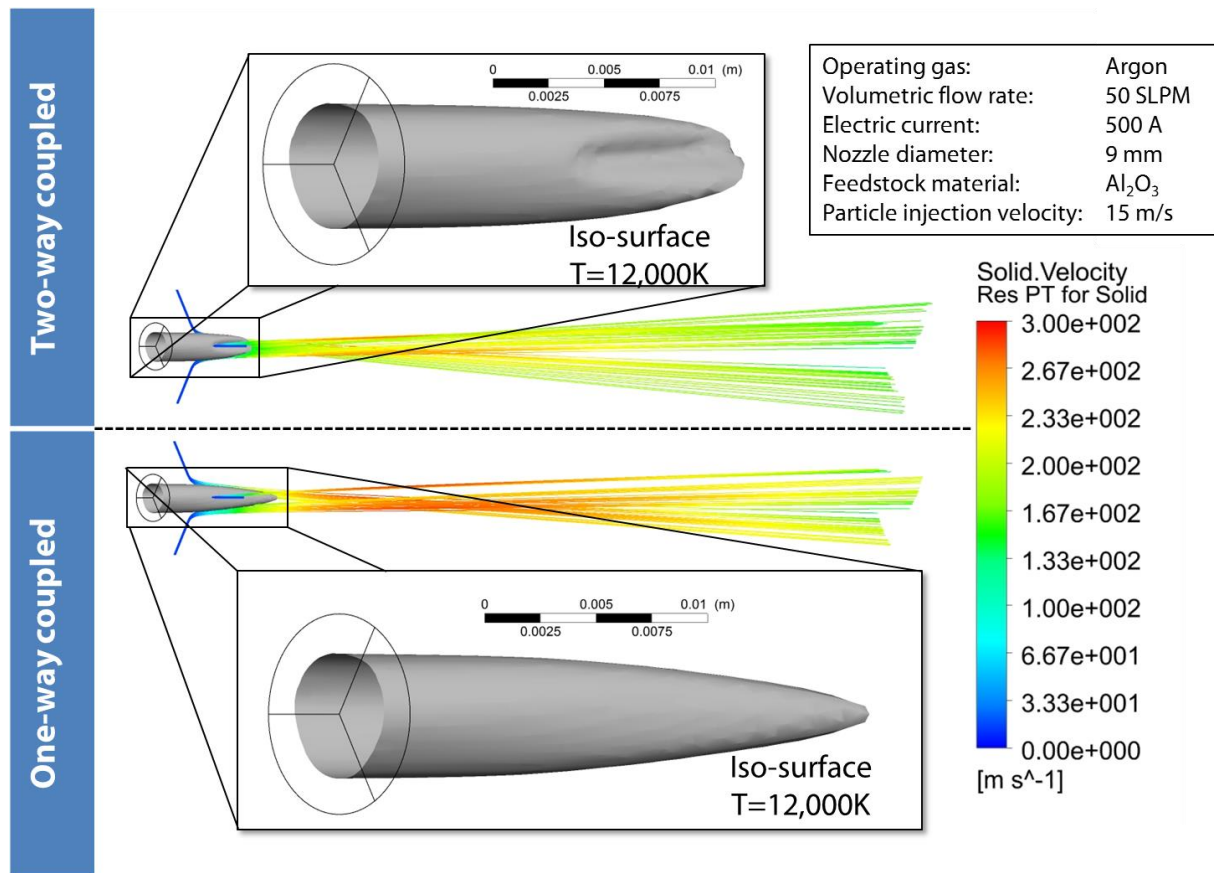
Figure 2. Comparison of calculated plasma gas temperatures and particle velocities in simulations which employ one-way and two-way coupling [36].

The results show that the particle injection clearly reduces the plasma temperatures leading to a slightly shorter plasma jet length. Moreover, it is apparent that in the injection region of the powder, the iso-surface representing the plasma temperatures at $T = 12,000$ K exhibits a distorted profile. This implies that the injected powder particles cool down the plasma jet in this region significantly. Neglecting the reduction of the plasma jet temperatures due to this effect causes in turn that the calculations of the particle in-flight characteristics show significant errors. On the one hand, the calculated heat and mass transfer between plasma gas and particles as well as melting degrees of particles are directly affected from over-estimated plasma gas temperatures as depicted in equations (4), (8) and (9). On the other hand, the changing thermodynamic and transport properties of the plasma gas with over-estimated plasma gas temperatures indirectly influence the calculated impulse, heat and mass transfer between plasma gas and particles. As a result, particle velocities, temperatures and melting degrees calculated with the approaches "one-way" and "two-way coupling" exhibit significant differences. Figure 2 shows exemplarily the comparison of particle velocities and trajectories which are calculated with these approaches. As it is evident that the plasma jet and particle in-flight characteristics are significantly influenced by the injected particles, the one-way coupling simplification shall be avoided for an accurate description of the plasma-particle interaction in plasma spraying.

5. Conclusion
A comprehensive numerical model focusing on plasma-particle interaction in case of new generation multi-arc plasma spraying systems has not been developed in the literature yet. In this study, this has been realized on the example of plasma jet generated by a three-cathode plasma spraying system. The

developed model takes almost all relevant effects into account, including melting, re-solidification and physical evaporation of the particles. On the basis of this model, the significance of the often used assumption that the particle phase does not have a significant influence on the plasma jet characteristics is critically evaluated. It has been shown that this assumption leads to significant errors in calculated plasma and particle in-flight characteristics. Therefore, the so-called "one-way coupling" approach, which is based on the above-mentioned assumption, shall be avoided for an accurate numerical description of the plasma-particle interaction in plasma spraying.

Acknowledgements

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