CFD SIMULATION OF PARTICLE MOVEMENT DURING ATMOSPHERIC PLASMA SPRAYING

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ABSTRACT

Atmospheric Plasma Spraying (APS) is a powder based coating process with versatile applications in terms of functional layers like corrosion, wear resistant or thermal barrier coatings. However, the fundamental process interactions cannot fully be described and understood experimentally. Therefore, a supportive CFD model was carried out by use of ANSYS 19.0. In detail, the CFD model consists of direct coupled electromagnetic and hydrodynamic formalisms. The particle behaviour was described by a simple multiphase reaction routine. Based on the CFD model, the resulting temperature field and the particle behaviour can be investigated. Especially, the particle trajectory, which represents the particle dwell time in the plasma stream, is of special interest for the final APS coating. Therefore, the description of a stable heat source is of major priority. This work shows a promising approach to evaluate the above mentioned particle and plasma properties, supported by a systematic parameter investigation. The obtained and experimental validated data can be used for a better process understanding as well as for further process optimisation.

Keywords: Atmospheric Plasma Spraying, APS, Simulation of Thermal Spraying, CFD simulation of particle movement, Process optimisation due to numerical simulation, Particle movement, Particle tracking

INTRODUCTION

Thermal spraying processes share about 35% of all world-wide used functional coating technologies. Especially, industrial applications (chemical industry and engineering) led to an overall invested capital of 3.1 billion USD of thermal spraying with a mean growing rate of 12% p.a. [1]. Atmospheric Plasma Spraying (APS) is part of these thermal spraying processes and is distinguished by high flexibility and high deposition rates. Due to parameter management and suitable process gases and torch properties, various material types, like ceramics or high-melting metals can be processed. This leads to a variety of applications, which have been published in literature [2-4]. However, due to many parameter interactions, an accurate extrapolation of known parameter sets for introducing new materials is not possible. Therefore, a transient CFD simulation is a promising approach to highlight parameter interactions and investigate the APS process in more detail.

The scope of this work is a CFD based description of particle movement in correlation to parameter dependent quantity fields. This numerical method can be used for better process understanding and process optimisation. Especially, the layer morphology, which is directly linked to particle inflight reactions, can be further improved by CFD based parameter management. The CFD Simulation consist of three main components:

- Material data
- Torch geometry (mesh)
- MHD model, using Electric Potential Method

MATERIAL DATA

Precise material data is crucial to describe physical interaction due to numerical simulation. In case of APS, three different material data sets were carried out and are directly influencing the numerical results:

- Process gas properties and environment
- Material data of the solid compounds
- Powder material

Pure Argon is used as plasma and particle carrier gas. Therefore, chemical properties like molar mass and physical properties like electric or thermal conductivity, heat capacity and viscosity were set up as a function of temperature and pressure. The gas data was provided by [5] in 100K steps from 300K to 30,000K. These wide ranged parameter windows form the foundation for the plasma arc (PA) simulation. The mixture of plasma gas and environment (air at 25°C) was also considered in the simulation model by a scalar material mixture model.

The material data for all solid parts made from copper, tungsten and steel were extracted from the internal material database of ANSYS 19.0. Due to the overall low process temperatures (ideal cooling), no additional temperature dependence material data was considered.

The powder material is described by idealised particle Gauß-distribution. The material data, such as the powder melting or sublimation temperatures, were assumed to be constant. This approximation can be applied due to the interaction of high energy densities (Plasma arc) and small particle diameters of max. 80µm, which lead to a fast phase transformation (<0.5ms). Pure zinc particles with a mean particle size according to Figure 1a) were used for CFD Simulation. Figure 1 shows an idealized particle size distribution (red dashed line) and spherical Zn particles, observed by SEM investigation. The spherical shape was implemented into the CFD Simulation by introducing a mass point with specific properties like diameter, mass and phase transition temperature.

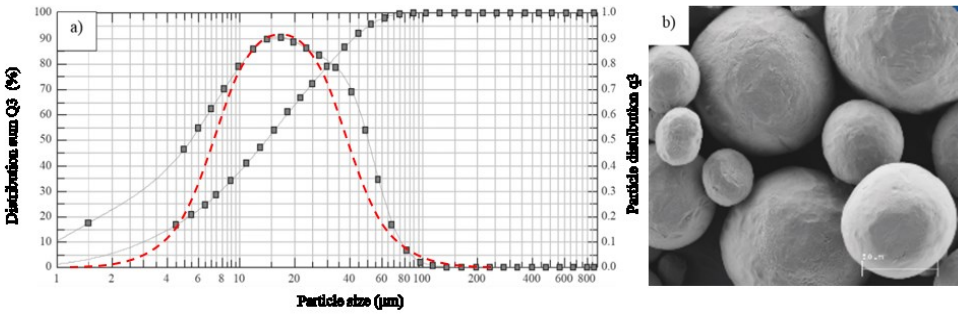

Fig. 1 a) Real particle size distribution of Zn powder. The red dashed line represents the idealized particle distribution, which was used for CFD Simulation b) SEM image of spherical shaped Zn particles

MESHING

The torch geometry was defined by use of CAD input data. Therefore, a full 3D mesh of the non-symmetrical Plasma torch (PT) with a total number of approximately 8 mil. elements was set-up. Due do complex body geometries, tetrahedral cell types were used. Regions of interests (ROI) and interfaces (IF) were systematically refined with a tetragonal element size of <0.2mm. To save computational time, the particular mesh size of ROIs and IF was increased stepwise by a factor of 1.3 using cylindrical coordinates. To describe the predominant molecular viscosity of a fluid flow at wall near regions and its interaction perpendicular to the wall surface [6], the local mesh was adapted (Fig. 2), whereby 3 mesh layers were applied parallel to the solid wall. The mesh quality was tested in terms of orthogonality, expansion and skewness by an internal software routine.

The final mesh consists of following solid and fluid components (IDs)

- Torch body (solid)
- Anode and cathode (solid)
- Supporting geometries (solid)
- Insulations (solid)
- Ambient (fluid)
- Main plasma gas flow channel and particle inlets (fluid)

Interface connections (e.g. Cathode – plasma gas flow channel) are considered by interface coupling during pre-processing. Therefore, both interfaces are selected manually and certain interface models (element connection, heat transfer,…) are taken into account. Figure 2 shows an example of mesh refining (ROI) and mesh adaption in a wall near region, which is crucial to generate the electric field and improves the convergence during iteration.

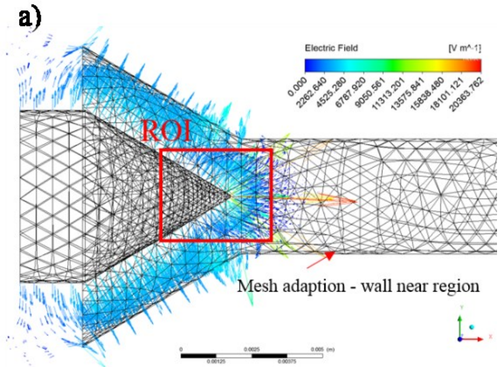

Fig. 2 Detail view of the cathodic near region. Mesh refining at the cathode tip, the interface and the flow channel (ROI). Mesh adaption in wall near region to display the boundary layer

MODELLING

To describe the particles' behaviour related to different physical influencing factors, a Computer Fluid Dynamics Simulation (CFD) is one possible approach. To define movement of complex particle flows mathematically, different numerical models are used to solve the partial non-linear differential equations. In case of APS the iterative solution of Navier-Stokes (momentum, heat and mass) and Maxwell equations (electromagnetic potentials) is the main goal during processing.

ELECTROMAGNETIC POTENTIAL

Physical effects like fluid flow, electricity, magnetism or turbulence, which are influencing the particle track, must be considered. Therefore, these interactions can be described by Electric Potential Method (EPM). Here, the current density is used to solve the electric potential equation by use of Ohm's law. The electric field $\vec{E}$ can be expressed as

$$\vec{E} = -\nabla\varphi - \frac{\partial\vec{A}}{\partial t} \quad (1)$$

Whereby $\frac{\partial\vec{A}}{\partial t}$ describes the change of vector potential over time and φ equals a scalar electric potential. For a static electric field the combined approach using Ohm's law and Maxwell equations can be expressed by the current density $\vec{J}$

$$\vec{J} = \sigma(-\nabla\varphi + (\vec{U}x\vec{B_0})) \quad (2)$$

$\vec{U}$… fluid velocity field
$\vec{B_0}$ … external imposed magnetic field

By applying a boundary condition for the electric potential φ and the principle of energy charge conservation $\nabla * \vec{J} = 0$, the basic equation to describe the electric potential can be written as

$$\nabla^2 \varphi = \Delta * (\vec{U} x \overrightarrow{B_0}) \tag{3}$$

The mathematic description of the electric potential (3) and the electric current density (Equation 2) can be used for magneto-hydrodynamic (MHD) coupling in a next step. By introducing additional terms to fluid momentum and energy equations, such as additional Lorentz Forces ($\vec{F} = \vec{J} x \vec{B}$) and Joule heating ($\vec{Q} = \frac{1}{\sigma} \vec{J} x \vec{J}$), the interactions of charged particles in an electromagnetic field can be calculated. Consequently, this approach can be used to describe the interactions of particles with a discrete charge density, particle velocity and a resulting Lorentz Force within a turbulent fluid flow.

TURBULENCE

The k-ε-model is a standard model to describe turbulent fluid flows with good accuracy and computational time [7]. The model itself is based on the eddy viscosity model, which describes the Reynold stresses by the phenomenon of molecular shear stresses. It describes the effect of different mechanisms (transport, diffusion, convection, dissipation,…) on the change of kinetic energy [8]. The turbulence model approach can be calculated as

$$\mu_t = \rho * c_\mu * \frac{k^2}{\varepsilon} \tag{4}$$

Where k represents the turbulent kinetic energy, ε the turbulent dissipation rate, c_μ is an empiric constant (value = 0.09) and ρ the density. The accuracy of the model in wall near regions is significantly reduced, due to dominance of molecular viscosity in those regions. Consequently, a dimensionless wall shear stress velocity u_r can be calculated, which is dependent of the dimensionless wall distance $y+$ according to equation

$$y^+ = \frac{y * u_r}{\vartheta} \tag{5}$$

Where ϑ is the fluid viscosity and y the wall distance. This wall function increases the accuracy of MHD coupling, and consequently improves the quality of final results.

PARTICLE INTERACTIONS

The interactions of acting particles are assumed by a set of mathematical models. The drag forces and the gas-particle were utilized by Schiller-Naumann model, which describes the interaction of primary and secondary phases of an Eulerian multiphase calculation. The rate of energy transfer (*Qpq*) was assumed as a function of temperature difference (6). The heat transfer coefficient is related to the Nusselt number Nu_p, which is calculated by Ranz-

Marshall correlation [9], [10]. This leads to the basic equation of the volumetric rate of energy transfer between 2 phases: p and q.

$$Qpq = hpq\left(Nu_p, \kappa, dp\right) * \Delta T(p, q) \quad (6)$$

Where hpq isvolumetric heat transfer coefficient between 2 different phases p and q. κ is the thermal conductivity and dp is the characteristic length. The elastic particle collision was described by Sommerfeld model, which is a stochastic model of two “virtual” collision partners.

All previously described models and the combination of energy, mass and transport equations complements the MHD model, which can now be used for a transient APS investigation.

RESULTS AND DISCUSSION

To describe the particle movement during the APS process, information about present physical quantities like pressure, temperature, velocity and turbulences is mandatory. The torch and the cathode is ideally cooled, which results in a 300K boundary condition at PT shell elements. Using the previously explained MHD model, transient quantities can be calculated.

TRANSIENT PHYSICAL QUANTITIES

In a first step, a defined parameter window for a steady-state calculations was set up. Table 1 shows the main variable parameters, which were used for the steady-state calculations, but also for further transient investigations. The steady-state result files were used as initial condition for the subsequent transient calculations. Especially, the interaction of inserted electric power and the particle size is of main interest.

Table 1 Investigated variable parameter window; Constant parameters: electric voltage, process gas flow (Argon), particle mass flow, working distance and particle carrier gas flow (Argon)

Parameters	Lower limit	Upper limit
Electric current (A)	60	200
Mean particle diameter (µm)	5	50

Due to fast particle speeds of >200m/s [1] (Fig. 3b), the total simulation time is fixed with 200ms and *Δt*=0.2ms. Figure 3 shows some representative examples using parameter set 2 (100A, 25µm) after 200ms.

However, parameter interactions were investigated in a previous work [11], but could also be confirmed by the MHD Simulation model within the investigated parameter window. As a result, the electric current was determined as the main influencing parameter concerning changing temperature and velocity fields, as well as particle properties. The parameter dependent, transient particle properties (Fig. 3c) can now be used to describe particle movement.

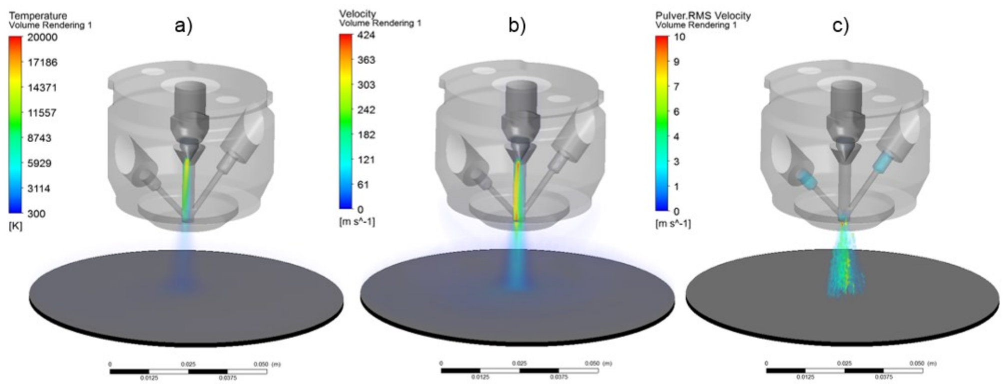

Fig. 3 Exemplary global results of transient physical quantities after 0.2s a) Plasma arc temperature, b) process gas speed, and c) powder flow speed

PARTICLE MOVEMENT

Based on the transient calculation of Gauß-distributed particle flows, single particles can now be traced and the particle movement can be investigated. Therefore, a random particle, which suffers elastic particle-particle and particle-wall interactions as well as physical interactions of turbulent fluid flows, is traced and recorded during post-processing. Figure 4a) shows 2 examples of particle movement at the interfacial area of powder inlet and main flow channel. Figure 4b) shows the resulting transient velocity vectors at the powder inlet and main flow channel interface.

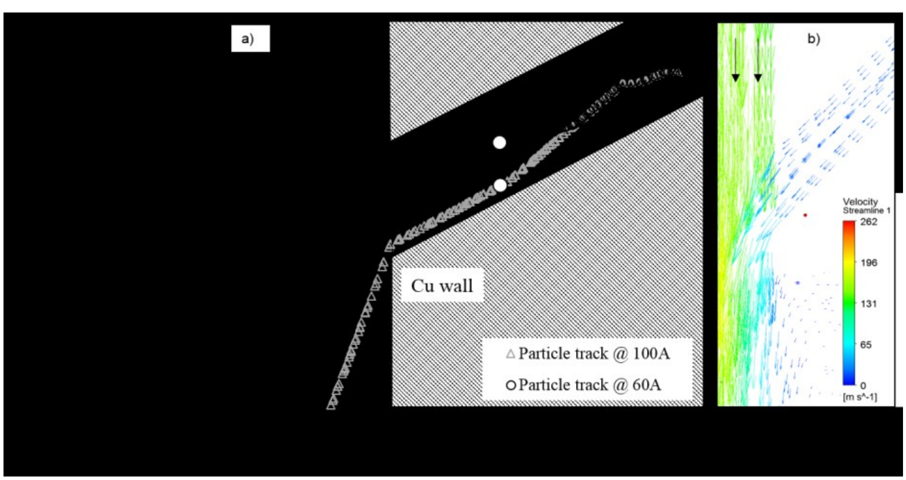

Fig. 4 a) Transient particle track of one representative particle using different parameter sets b) Vector plot of the local velocity field using standard parameters (100A)

Due to different primary currents the particle track differs. By increasing the electric current two main effects take place. First, the local gas velocity (main flow channel) increases, which leads to more pronounced velocity-vector orientation in z-coordinate direction and respectively a reduction of the particle dwell time. Second, due to higher plasma temperatures, the resulting particle temperature increases. However, these combined effects are influencing the particle movement, and consequently correlate with the inflight particle properties. As a result, various physical properties can be investigated: e.g. the particle phase fraction (Zn).

PARTICLE PHASE FRACTION

The calculated particle track gives insight about important coating related phenomena. Especially, the correlation of the particle travel path and the phase state of the tracked particle is of main interest for the APS process and the final APS coating. Therefore, a Liquid2Solid (L2S) subroutine was implemented in the MHD model, in order to calculate the liquid particle fractions as a function of process dependant transient physical quantities, e.g. particle velocity, mass flow rate, temperature field and pressure. The foundation of the simple L2S subroutine is the definition of different phase transformation points. As mentioned above, a constant melting temperature of T_m=692.45K can be assumed for all Zn particles. This melting temperature represents the main phase transition point during particle movement. Other phase transformations like particle agglomeration, solidification and sublimation were neglected in the L2S routine.

A typical application for APS is the local deposition of Zn based corrosion resistance coatings onto steel sheets. Therefore, a combined approach of an experimental parameter investigation and CFD Simulation is one possibility to improve the Zn coating properties. Table 2 shows 4 representative parameter sets.

Table 2 Investigated parameter sets. Const. parameters: Working distance=30mm, Powder mass flow=5g/min, Particle carrier gas flow=5l/min, Powder material=Zn

	Electric current (A)	Plasma gas flow (l/min)	Particle size (µm)
Parameter set 1	60	10	5
Parameter set 2	200	10	5
Parameter set 3	200	10	50
Parameter set 4	80	12	25

Figure 5 shows the correlation of the phase fraction of a random Zn particle and the calculated particle travel path for all specific parameter sets.

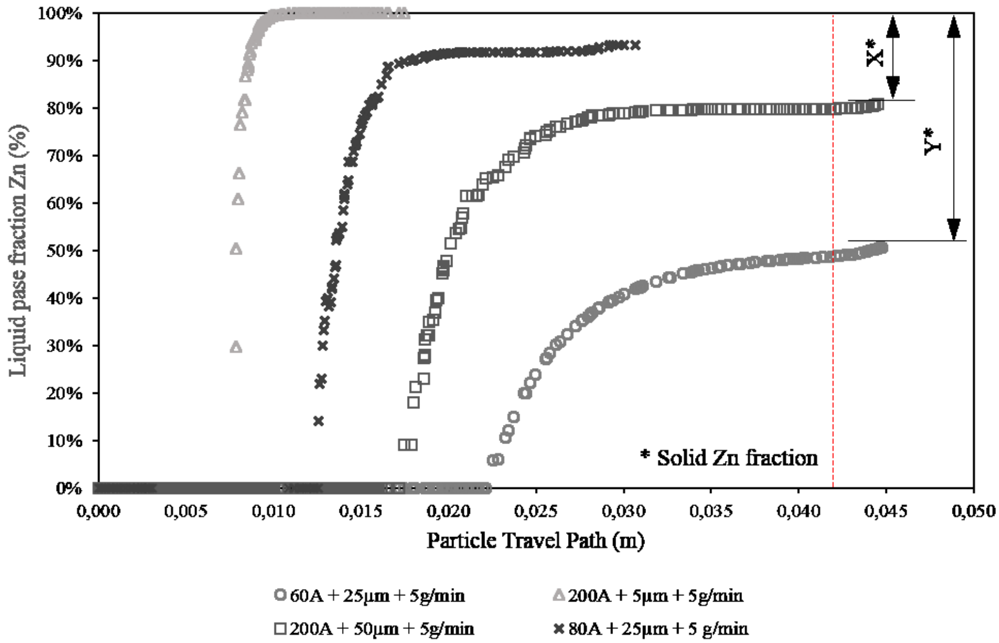

Fig. 5 Correlation of the tracked particle path and the phase fraction of Zinc. Different parameter set were investigated by experiment and simulation; Red dashed line represents the shortest possible particle track, due to PT geometry

However, while one base criteria for homogenous APS coatings is the liquid phase fraction should be near 100%, the remaining solid fraction of Zn particles (X^* and Y^*) can be calculated during particle flight. Liquid Zn droplets lead to a more pronounced splat formation and to more compact APS coatings respectively [12]. Representative cross sections of the deposited APS coatings were investigated by light optical microscopy (LOM).

Figure 6a) shows typical irregularities like void formation, increased porosity, irregular coating thicknesses and a decrease of inter-particle adhesion forces. These irregularities occurred predominantly near semi-molten particle boundaries, due to incorrect process parameter setting. Figure 6 b) shows a representative cross section of the Zn coating, which was deposited using a MHD computed parameter set (parameter set 4). As a result, predominant solid particles could be avoided and the amount of irregularities could be significantly reduced.

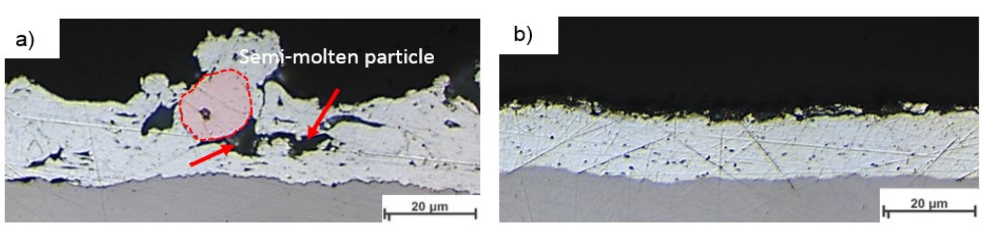

Fig. 6 LOM investigation of two representative cross sections of a Zn layer on a steel substrate a) Local void formation of particle near region and irregular surface morphology, due to semi-molten particles – Parameter set 1 b) Zn coating deposited with parameter set 4

SUMMARY AND CONCLUSION

The present, physical based MHD simulation model can be used for optimising the deposition process. First, transient physical quantities like temperature, velocity or pressure were calculated. These quantities give an insight about parameter interactions and physical loads during APS, depending on the PT geometry. Second, these quantities act as an initial condition for the subsequent particle track calculation. Therefore, one random particle is tracked during its' flight through the powder inlets and the main flow channels, interacting with the previously described physical quantity fields. As a result, the particle track for each involving particle could be calculated. Third, the interaction of particle moving and particle phase fraction (Zn) was investigated.

The MHD Simulation of the APS process led to some interesting findings:

- The combined approach of particle movement simulation and the implemented S2L routine allows process and parameter optimisation. Therefore, the liquid phase fraction of a particle, which correlates with splat formation, can be calculated. As a result, a reduction of semi molten particles within the Zn coating could be achieved by use of the MHD simulation model. Consequently, the amount of irregularities could be significantly reduced, which could also be confirmed by experimental investigation.
- The simulation model can be used to investigate and validate new powder materials. Here, the prediction of the coating morphology and the deposition efficiency are in the main focus. The simulation results correlate with the microscopic analyses.
- The numerical simulation can be used to improve the PT or cathode design. Here, the formation of transient temperature fields and the resulting particle movement is of major interest.

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