Chapter from the book *Numerical Simulations - Applications, Examples and Theory*

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1. Introduction

Atmospheric pressure plasma spraying is widely used to produce various coatings, especially hard ceramic coatings for wear and corrosion protection and thermal barrier function, porous catalytic coatings for environment control and protection, hydrophobic coatings, etc. The plasma spraying process uses a DC electric arc to generate a jet of high temperature ionized plasma gas, which acts as the spraying heat source. The sprayed material, in powder form, is carried into the plasma jet where it is heated, partially or fully melted and propelled towards the substrate. The properties of the produced coating are dependent on the feedstock material, the thermal spray process and application parameters, and post treatment of the coating. However, the influence of flow and particle temperature and velocity on coatings characteristics, its adherence to the substrate, reproducibility of its properties and quality is not clearly established [Fouchais et al., 2006]. Generally, to correlate coating properties to flow parameters and particle in-flight characteristics experimental procedure is used. To monitoring the whole plasma spraying process (plasma jet generation, powder injection, formation of the coating) same techniques, as plasma computer tomography (PCT), particle shape imaging (PST), particle flux imaging (PFI) [Landes, 2006] are used. Such techniques are expensive and complicate for use in industry. Numerical investigations of plasma spray process generally is focused on investigation of heat transfer between plasma jet and surface [Garbero et al., 2006], substrate temperature influence on coatings morphology, adhesion, chemical processes between substrate material and deposited material [Yeh, 2006, Kersten et al., 2001].

In this paper, by means of Jets&Poudres software [Delluc et al., 2003], a numerical simulation of interaction of plasma jet and dispersed particles was investigated. Simulation results were compared with experimental data.

2. Methodology

Numerical research of two-phase high temperature jet was carried out using “Jets&Poudres” software [Delluc et al., 2003], created on the basis of General Mixing (Gemmix) software improved by using thermodynamic and transport properties closely related to the local temperature and composition of the plasma. For a particle in a plasma
jet, two characteristics are studied: motion (trajectory, velocity) and thermal evolution (temperature, physical state, heat flux). Thermodynamic and transport properties of the gases are obtained from the T&TWinner data base [http://ttwinner.free.fr]. The coating material particle characteristics are also available as a data base. Calculations are carried out for air plasma at atmospheric pressure flowing from jet reactor exhaust nozzle to substratum. When the parameters of plasma jet are achieved as desirable, hard spherical dispersed particles are injected into the flow. Performing modeling and calculating the deformations of the plasma jet thermo fields are disregarded, inlet profiles of temperature and velocity are rectangular shaped and correspond to estimated experimental data [Kezelis et al., 1996]. Plasma jet flows in one direction and the flow is stable, without recirculation and diffusion effects. The numerical simulation results were compared with experimental data.

Experimental plasma spraying system [Valincius et al., 2003] consists of linear DC plasma generator (PG) 30 - 40 kW of power with hot cathode and step-formed anode, plasmachemical reactor, systems of power supply and regulation, PG cooling, feeding and dosing. The operational characteristics of plasma generator are represented in [Valincius et al., 2004].

| Regime | I  | II | III |
|--------|----|----|-----|
| P, kW  | 49 | 49 | 49  |
| G, gs⁻¹| 5,5| 5,5| 5,5 |
| G(H₂), gs⁻¹| 0 | 0,1| 0,15|
| T, K  | 2700 | 3400 | 3770 |
| X, mm | 70 | 70 | 70 |
| V, m/s | 1000 | 1400 | 1580 |

Table 1. Plasma spraying regimes for Al₂O₃ films deposition

During plasma spraying experiments the operating conditions of plasma torch were maintained constant. The capacity of plasma torch, total mass flow of air, cooling water and it temperature were measured and from this data plasma jet temperature calculated (see Table 1.). Injection of hydrogen was used to vary outlet plasma jet temperature and velocity, while plasma torch parameter was stable. Powder injection was provided into reactor, which was connected directly to plasma torch anode. Micrographs of the Al₂O₃ powder and sprayed films morphologies were collected using a scanning electron microscope and optical microscope. The sprayed particles were collected into distilled water. These granules can be industrially used as high temperature insulating material. Other primary data (determined by experiments) are as follows: flow outlet nozzle diameter d = 10⁻² m; the diameter of particles 50 - 70 µm; the exhaust jet is surrounded by air of unrestricted space. The computing domain is a cylinder-shaped space covered with a set of meshes of a grid. The diameter of the computing domain is 200 mm and the total number of variable size geometrical grids is approximately 300000. This is described in detail in [Valinciute, 2007].

3. Results

After mixing with plasma jet, solid particles need some time to heat and at the start their temperature is lower than the temperature of plasma gas. Particles are small-sized and quickly heat up; they are heated in plasma jet by convection, whereas inside particles the
heat is transferred by conduction. As it can be seen from Fig. 1(a), the temperature of dispersed particles near substratum surface exceeds average temperature of gas jet and is $1200 - 1600$ K.

![Graph of temperatures](image1)

![Graph of velocities](image2)

Fig. 1. Distribution of temperatures (a) and velocities (b) of Al$_2$O$_3$ particles and plasma jet determined by measurements along the spraying distance. 1, 2 show plasma jet experimental and numerical simulation results respectively, 3, 4 and 5 represent particles of 75, 50 and 35 µm in diameter respectively. x/d is a dimensionless distance.

As can be seen from Fig. 1b, velocity of dispersed particles near the covering surface exceeds average gas jet velocity and depending on the sizes of particle reaches $150 - 320$ m s$^{-1}$. The smallest particles achieve higher speed than bigger ones, so, the deciding factor of velocity changes is a resistance force. The velocity of particles stabilizes at x/d = 7 and then the size of particles almost has no significant influence. The surface of substratum at the distance x/d = 8 - 12 will be hit stable force by the jet stream and the value of kinetic energy is ultimate. Figure 2 represents the proportional distribution of plasma jet and dispersed ceramic particles temperatures, measured or calculated by different authors [Delluc et al., www.intechopen.com]
The trajectories of plasma flow are very similar and have a near agreement. Some differences at the end of travel distance can be observed. Disagreement occurs due to different experimental set-up operating conditions, numerical simulation options, and plasma spraying process regimes.

Fig. 2. Nondimensional distributions of plasma temperature (1 - calculated with “Jets&Poudres” by other authors [Delluc et al., 2005], 3 - our experimental research, 4 - calculated with “Jets&Poudres”, 6 - calculated by other authors using other numerical models [Klocker et al., 2001]) and ceramic 50 µm particles’ temperature (2 calculated with “Jets&Poudres” by other authors [Delluc et al., 2005], 5 - our calculation with “Jets&Poudres”)

Fig. 3. Variation of Reynolds number along spraying distance

Variation of curve Reynolds number (Re) along flow axis is presented in Fig. 3. In our case, for the regime 1 in Table 1 the value of Re varies from 2 to 12. The largest value of Re is found near the outlet. Since jet mixes with the ambient air and is interrupted, flow becomes...
unstable. On further gas in the jet cools down and slightly stabilizes itself. At a distance $x/d = 3$ from exhaust nozzle, Re value slightly increases since in this period the jet is slightly disturbed. At this moment a very intensive melting of particles occurs and recirculation zone appears. At $x/d = 8 – 9$ from exhaust nozzle a particle does not melt and flow stabilizes, whereas Re number obtains a steady value.

![Graph showing the dependence of melting degree of 50 μm Al₂O₃ particle from spraying distance](image1)

**Fig. 4.** Dependence of melting degree of 50 μm Al₂O₃ particle from spraying distance

**Fig. 5.** SEM micrographs of initial powder (a) and after passing through the plasma jet: (b) at $x/d = 35-40$ mm outlet form nozzle, (c) the granules produced at $x/d = 10$ from outlet nozzle

Intensity of particle’s melting ($Y, \%$) in jet depending on travel distance along the flow axis is presented in Fig. 4. The interaction between high temperature jet and injected particles begins immediately. The particle, injected into plasma jet, passes three main flow zones until it reaches a fixed substratum: heating of the particle, its melting, and stable flow. As can be seen from results, initial heating period of the particle continues to $x/d = 2.7 – 3$. During this time the largest part of plasma energy is used for heating the particle. When particle is heated up, it begins to melt due to physical and chemical conversions inside it. Temperature of particle gradually rises and melting rapidly proceeds. The most rapid melting occurs at distance $x/d = 3 – 8$ from exhaust nozzle and this is the second melting zone of particle. The practical usability of calculation results has been verified by comparing the simulation data with experiments.

![Image showing SEM micrographs](image2)
[Valatkevicius et al., 2003, Brinkiene et al., 2005]. Morphologies of plasma-sprayed Al$_2$O$_3$ powders during the II regime (Table 1) are shown in Fig. 5. As observed by scanning electron microscopy, the initial powder is in the form of agglomerates with wide size distribution. To determine the melting degree, shape, and size of sprayed particles, they have been collected into distilled water at different distances from outlet nozzle. After passing x/d = 3.5 - 4, the particles appear partially melted (Fig. 5(b)). During the melting of initial particles of 100 µm in diameter the plasma spray pyrolysis process occurred. Dispersed particles of Al$_2$O$_3$ injected into arc column showed a very fast bulk melting and then very fast particle surface cooling. Further from plasma torch nozzle to the substratum the particles turn into very large granules with the diameter of 150 - 200 µm (Fig. 5(c)). When the coatings are produced, particles resolve into small fragments on their way and splash on the surface of substratum. Sharp edges of particles become round and the surface of coating becomes fine and smooth (Fig. 6). Applying the I regime of plasma generator (see Table 1) and regulating the working gas flow, PG arc current, spray distance, and at initial diameter of 30 - 50 µm of dispersed particles, the porous coatings with large free surface for catalytic application (Fig. 6(c, d)) are obtained. Applying the III regime, dense thin films for protective purposes could be deposited (Fig. 6(a, b)). In the latter case the plasma spray pyrolysis effect has occurred and initial dispersed particles have broken up into a large amount of fragments. Consequently the grains of plasma sprayed coatings were smaller than 5 µm.

![SEM micrographs of dense and porous plasma sprayed alumina coatings](https://www.intechopen.com)

Fig. 6. SEM micrographs of dense and porous plasma sprayed alumina coatings: (a, c) surface morphology, (b, d) cross-section pictures
4. Conclusions

Plasma spraying technology at atmospheric pressure offers the possibility to obtain microsized particles, granules, and coatings from inorganic metal oxides with controlled characteristics for special application. Plasma jet-particle interaction lasts for about 1.2 ms and strongly depends on jet temperature, velocity, and particle's mass.

While moving in a jet, the ceramic particle is heated, melted, and splats on the substratum. The most intense melting of particles occurs at \( x/d = 3.8 \) from exhaust nozzle. Velocity of the particle near the substrate exceeds average plasma jet velocity and depending on the diameter of particle reaches up to 150 - 320 ms\(^{-1}\). At \( x/d = 8 - 12 \) from exhaust nozzle the dispersed particles' flow is steady, whereas the value of kinetic energy is ultimate.

The numerical calculation data shows that the applied numerical model of two-phase high temperature jet calculation is in good agreement with experimental data and could be used to determine the optimal plasma spray parameters for coatings with desirable characteristics. The grain size of plasma sprayed coatings is smaller than 5 \( \mu \)m.

5. Acknowledgement

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This book will interest researchers, scientists, engineers and graduate students in many disciplines, who make use of mathematical modeling and computer simulation. Although it represents only a small sample of the research activity on numerical simulations, the book will certainly serve as a valuable tool for researchers interested in getting involved in this multidisciplinary field. It will be useful to encourage further experimental and theoretical researches in the above mentioned areas of numerical simulation.

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