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Numerical approach and optimization of the combustion and gas dynamics in High Velocity Suspension Flame Spraying (HVSFS)

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ABSTRACT

The interest in submicron and nano-structured layers applied by thermal spray technologies on different surfaces has been significantly increased during the last decade. Conventional HVOF spraying processes are not suitable to achieve submicron and nano-particles. Therefore, High Velocity Suspension Flame Spraying (HVSFS) has been developed for the processing of nano-structured spray material to achieve dense surface layers in supersonic mode with a refined micro- or nano-structure, from which superior mechanical and physical properties are expected.

However, the chemical and thermodynamic phenomena occurring in the HVSFS reacting flow field are a challenging, multidisciplinary issue. This study is intended to analyze and understand the HVSFS combustion and flow dynamic system on the basis of a CFD model and numerical calculation. The final aim is an optimization of the process parameters by variations during simulation experiments.

1. Introduction

One of the great challenges in thermal spray technologies to date is the manufacturing of nanostructured coatings and functional surfaces. This development is motivated by the discovery that properties of such materials are superior to those of conventional metal or ceramic coating materials, including greater strength, hardness, ductility, and sinterability [1]. Otherwise, reducing the grain sizes of coating materials from conventional levels (i.e., <10 µm in metals and <1–2 µm in ceramics) to nanostructured levels (i.e., <100 nm) can considerably enhance its mechanical strength and hardness [2,3].

Different spray techniques are usually employed to made nanostructured coating materials. One of the widely employed processes consists to use regular powder feeders, in this technique the nanosized materials are agglomerated via spray-drying and then partially sintered into microscopic particles. This process is usually employed when very fine materials such as nanostructured ceramic or cermets powders are to be thermally sprayed [4–6].

Powders composed of nanosized particles (<100 nm) are extremely critical in handling and processing. The potential of these materials to pose risks to health is not yet fully examined and well understood. Nanoscaled particles easily distribute in air, penetrate the human skin or pass through the respiratory tract and the lungs, finally entering the blood circuit. In resume, there is no way to feed submicrometer or even nanopowders with conventional powder feeder techniques, not only that safety aspect would forbid any refilling, cleaning, etc. under habitual conditions, but mechanical feeding is virtually impossible due to the strong agglomeration of the powder particles that prevents a good flowability. Processing the powder in the form of a suspension (in aqueous or organic solvent) solves those problems, the handling is facilitated and feeding of the liquid can be realized with quite simple thermal spray techniques [1].

Some of these techniques are the suspension plasma spraying (SPS) or the solution precursor plasma spraying (SPPS), both processes allowing manufacturing finely structured layers of thicknesses varying between a few micrometers up to a few hundred of micrometers. The liquid solvent using in this technique permits to inject particles in the thermal flow (due to their small size, a carrier gas cannot play this role) whose finally heated, accelerated and sprayed onto the substrate. Compared to conventional plasma spraying, SPS and SPPS are by far more complex because fragmentation and vaporization of the liquid solvent control the coating build-up mechanisms [7–9]. For example by the processing of nanostructured TiO_2 (anatase) powder, the nanoparticle agglomerates produced by such evaporation are therefore largely unmelted, so that the coatings retain much nanostructured anatase and show abundant fine porosity. These characteristics are desirable for enhanced photocatalytic activity [10,11], but seem unfavorable for other applications, like sliding wear protection. Another intrinsic difficulty of SPS is the radial injection required by most DC plasma

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torches: this implies that the injection system must be carefully designed, because, if too many droplets cannot reach the plasma core, highly defective coatings are produced [12]. Voltage fluctuations can also be detrimental to the stability of the SPS process [12].

The focus of research on nanostructured materials is now shifting from powder synthesis to processing of nanostructured coatings using supersonic thermal spray processes. This new approach, based on the conventional high velocity oxide fuel (HVOF) thermal spray, consists to spray submicron or nanoparticles with hypersonic speed with the aim to form thin and dense coating layers [1,13,14]. The HVOF spraying is a long established technique besides flame, arc wire or atmospheric plasma spraying. The HVOF thermal spray process is characterized by very high gas and particle velocities, followed by relatively low gas temperatures, as compared to plasma spray processes. Mainly ceramic coatings applied via HVOF have been extensively improved as corrosion-resistant, anti-corrosion, anti-adhesion, wear-resistant surface layers, or combinations of these to extend product life, to increase performance and to reduce time and costs. However, the conventional HVOF thermal spray system is only suitable for the processing of micro-scale powders and has distinct limitations in powder size due to powder supply and several difficulties mentioned above [15,16]. This means that some adaptations of the HVOF process are needed for the processing of nano-scale powders.

High Velocity Suspension Flame Spraying (HVSFS) compared to SPS and SPPS also use a liquid solvent as carrier fluid to process nano-scale materials. In those techniques (SPS, SPPS, HVSFS) the coatings material is processing in the form of a suspension. Suspension is a heterogeneous mixture containing solid particles and a solution. In our institute (IFKB) various suspensions were fabricated using aqueous and organic solvents (ethanol, isopropanol). This consist to mix the powders with the solvent and stirred together with appropriate dispersing agents (i.e. as Trusan 471 from Trukem) and stabilizers (citric acid, acetic acid) to ensure stable dispersions. The solid contents were in the range of 10–15 wt.%. Distilled water, ethanol and isopropanol were used as solvents. Subsequently the suspensions were ground using an attrition mill (Dispermat SL, Getzmann) to prevent any formation of agglomerates. After this procedure all suspensions showed adequate stability and were ready for processing [14].

By HVSFS, the suspension is injected directly (centered and in axial direction) into the combustion chamber of the operation Torch with the liquid contributing to the reaction enthalpy of the combustion process [14]. The suspension has to be delivered against the combustion chamber pressure, just like in standard powder feeding but with a special feeder system. A pressure vessel (maximum load 10 bar) holding the suspension that is operated with compressed nitrogen gas is use at IFKB for experimental processing of HVSFS. This feeder technique has been made to transport suspension and to prevent it from sedimentation in less stable case by using i.e. a stirring device. A valve allows switching between suspension and a flushing gas or solvent to prevent clogging of the suspension line when starting or terminating spray operation [1,13,14]. This injection process shows some difficulties compared to conventional powder feeding in terms of pressure distribution and also the possibility of composition variations and in-situ change of the composition. Therefore, an optimization of the injection behavior of suspensions was done in earlier work by modification of the nozzle geometry [1,13,14].

Using a solution as carrier fluid for nanostructured materials processing in thermal spray systems features some thermophysical and thermochemical changes of the new HVSFS process compared to the standard HVOF process. These include the existence of a third phase (liquid), its evaporation and combustion including a cooling effect in the spray torch, and also the resulting particle morphologies (agglomeration) are different from conventional HVOF processes [9].

The chemical, thermal, thermophysical, and morphological states of the suspension and the particles during the process ultimately determine the coating microstructure and its macroscopic properties. Parameters such as droplet size, injection velocity, the location of solution evaporation and initial combustion, flame temperature and velocity fields in the combustion chamber and expansion nozzle can all have significant influences on the final outcome in terms of the coating structure and its properties.

Regarding the thermophysical and thermochemical properties of HVSFS, the following phenomena have to be considered during analysis of the processes in the combustion chamber:

- combustion of the fuel gas (premixed oxygen/propane),
- heat, momentum and mass transfer between the flame (propane flame) and the suspension droplets (organic solvent and particles), and
- evaporation and combustion of the suspension organic solvent (non-premixed ethanol combustion).

In this work, 3D modeling and analysis of the combustion and gas dynamic phenomena of the HVSFS process, including the modeling of ethanol evaporation and analysis of the interaction mechanisms between gas and liquid as well as between gas and particles, is performed at the example of an industrial TopGun-G torch. The thermal and flow fields of gas are solved by an Eulerian approach and the particle velocity, temperature and degree of melting by a Lagrangian approach. Regarding the gas dynamics, the Reynolds and Favre-averaged Navier–Stokes equations implemented on the commercial CFD software ANSYS-CFX are solved. Due to high Reynolds numbers and large pressure gradients in the combustion chamber and in the nozzle, the $\kappa\varepsilon$-turbulence model is used with the scalable turbulent wall function in order to implement wall friction and heat transfer into the model. The eddy dissipation model [15,17,18], which assumes that the reaction rate is limited by the turbulent mixing rate, is employed to model the chemistry reaction occurring during premixed combustion (propane). An Antoine equation assumption is utilized in the liquid evaporation model [9] for determining the liquid droplet properties (temperature, velocity, diameter, etc.) during the energy transfer in the combustion chamber. After liquid evaporation, the finite rate chemistry model [19] is used to solve the rate of progress of elementary reactions taking place during diffusion combustion (non-premixed ethanol vapor). Particle breakup is modeled using the Blob method for disperse droplets and the ETAP method for disperse solids according to the Weber and Reynolds number of each particle. The Blob method is one of the simplest and most popular approaches to define the injection conditions of droplets. In this approach, it is assumed that a detailed description of the atomization and breakup processes within the primary breakup zone of the spray is not required. Spherical droplets with uniform size, $d_{\mathrm{p}} = d_{\mathrm{nozzle}}$ are injected that are subject to aerodynamic induced secondary breakup. The spray angle is either known or can be determined from empirical correlations. The “blob-method” does not require any special settings but is the default injection approach in this process. A uniform diameter model was used for the ethanol droplets and a discrete diameter distribution model was used for the particle size distribution of the solid particles (titania powder in micro and nano scale). This parameter enables verification of the powder size distribution in the model. Two-way coupling was used for the energy and mass transfer between gas and liquid, while one-way coupling was used during modeling the thermal and kinetic energy transfer from gas to solid particles, assuming that the particles have no distinct influence on the gas properties [15–17].

This study is based on and continues the numerical analysis of the conventional HVOF thermal spray process as described in earlier work [15]. There, a detailed numerical description of the fluid mechanics, the transport phenomena and the flow instabilities due to high pressure gradients is given for the free jet area (spray distance between torch outlet and the substrate), which was simplified in the