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Numerical investigation of combustion and liquid feedstock in high velocity suspension flame spraying process

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Over the last decade the interest in thick nano-structured layers has been increasingly growing. Several new applications, including nanostructured thermoelectric coatings, thermally sprayed photovoltaic systems and solid oxide fuel cells, require reduction of micro-cracking, resistance to thermal shock and/or controlled porosity. The high velocity suspension flame spray (HVSFS) is a promising method to prepare advanced materials from nano-sized particles with unique properties. However, compared to the conventional thermal spray, HVSFS is by far more complex and difficult to control because the liquid feedstock phase undergoes aerodynamic break up and vaporization. The effects of suspension droplet size, injection velocity and mass flow rate were parametrically studied and the results were compared for axial, transverse and external injection. The model consists of several sub-models that include pre-mixed combustion of propane-oxygen, non-premixed ethanol–oxygen combustion, modeling aerodynamic droplet break-up and evaporation, heat and mass transfer between liquid droplets and gas phase. Thereby, the models are giving a detailed description of the relevant set of parameters and suggest a set of optimum spray conditions serving as a fundamental reference to further develop the technology.

1. Introduction

In recent years, the use of liquid feedstock as carrier of nano-sized powders (<100 nm) in thermal spray processes has been started as an outstanding vehicle for the deposition of submicron-sized particles [1–3]. The consistently high level of interest in the field of suspension thermal spraying (STS) and solution precursor thermal spraying (SPTS) is reflected by the number of review papers published [4–8]. In fact, coatings made of nano-particles have shown outstanding characteristics in a vast range of applications, I.e., aerospace, turbomachinery blades, machining, etc. Among improved advantages of nano-sized coatings are better corrosion protection, augmentation of composite strength [9], fire protection, water resistance [10], and high endurance [11]. Liquid spray in general could offer unprecedented opportunities in designing and fabricating increasingly complex material architectures with controlled and hierarchical microstructures. Recent examples include the fabrication of thermoelectric modules and solar cells made from thermally sprayed silicon wafers.

One of the major challenges in processing nano-meter sized particles by high velocity thermal spraying is their precise injection into the core of the high-enthalpy flow. As such, decreasing the particle average size down to the nanometer scale requires a significantly higher injection force equal to that imparted to them by the flow. In turn, the increased cold carrier gas flow rate requirement disrupts the high-enthalpy flow [12,13]. A first option to circumvent such a drawback is to agglomerate nanometer-sized particles into micrometer-sized agglomerates and to inject them using a conventional route based on carrier gas [14]. Evidently, the lower density and lower thermal conductivity of those particles has to be taken into account when adjusting the torch operating parameters since heat is diffused slower within such agglomerated particles compared to the fully dense particles of the same diameter. Although particle handling is easier, another disadvantage of such an approach is that the coating does not exhibit a complete nano-mater-sized structure. To overcome the above mentioned problems, suspension of nano-particles in either aqueous or organic solvent has recently being employed, which allows using very fine particles for thermal spraying coatings achieving in this way full coating nanostructure[2,3,12,15–19].

High velocity suspension flame spraying (HVSFS) is based on the conventional high velocity oxy-fuel (HVOF) thermal spraying process and was developed with the aim of spraying submicron or nanoparticles suspensions with hypersonic speed to deposit thin and very dense coatings achieved through experimental studies [2,3,19–21]. HVSFS uses a liquid solvent as carrier fluid to process nano-scale materials, in which the coating material is in the form of a suspension. A suspension is a heterogeneous mixture containing solid particles and a solution or solvent (water, ethanol, or isopropanol) [18]. When the suspension is made of water, poor coatings are obtained due to insufficient flame enthalpy. Much better results are obtained with ethanol, but even a low percentage of water in ethanol drastically cools the flame. Injecting combustible

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liquids raises the combustion chamber pressure, resulting in instabilities in the acetylene flow (acetylene–oxygen giving the highest combustion temperature). Thus propane and ethane are used [21] to achieve stable flames with the Top-Gun system while Oberste-Berghaus et al. [20] have chosen propylene with the DJ2700 system.

There are, however, very limited numbers of numerical studies in the literature about HVSFS process since most of the work undertaken to date in this field is mostly focused on plasma and HVOF spraying processes. To best of our knowledge, there is only one numerical investigation of HVSFS process conducted by Dongmo et al. [22]. The work is 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, performed at the example of an industrial TopGun-G torch. An Eulerian approach is used to solve the thermal and flow fields of gas while the particle trajectory is modeled in a Lagrangian fashion. The turbulence model is the k-ε and the eddy dissipation and the finite rate chemistry models are used to solve pre-mixed propane/oxygen and non-premixed ethanol/oxygen combustions respectively. A liquid evaporation model is employed to predict heat and mass transfer between two phases. The model uses two mass transfer correlations depending on whether the droplet is above or below the boiling point. The boiling point is determined through an Antoine equation which is a vapor pressure equation that describes the relation between vapor pressure and temperature for pure components. Finally, it is mentioned that particle break up is modeled using the Blob method for disperse droplets and ETAP method for disperse solids according to Weber and Reynolds number of each particle. The results of modeling showed that the ethanol evaporation and combustion take place in the barrel of the gun lead to highly cooling the gas temperature and disturb the energy balance. Ideally cooling of the gas temperature should be minimized to a very little amount and occur inside a combustion chamber to contribute the enthalpy of combustion and not imbalance the thermal and flow fields of HVSFS process. However, this study does not analyze the secondary break up of liquid droplets, which is found in the present work to play an important role. Furthermore the evaporation effects on gas dynamics are not examined thoroughly. Compressibility effect and shock diamonds are not captured outside the gun and only axial injection scheme is used for the analysis of droplet injection.

HVSFS process compared to HVOF is more complex. The chemical, thermal, thermophysical, and morphological states of the suspension and 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, mass flow rate of liquid feedstock, location of injection point, flame temperature and velocity fields in the combustion chamber and expansion nozzle can all have significant influence on the final outcome in terms of the coating structure and its properties.

This paper, therefore, primarily aims to deepen the knowledge on such multidisciplinary process and to address current drawbacks mainly due to cooling effects and reduction of the overall performance of the spray torch. The detailed parametric study includes modeling and analysis of premixed (propane/oxygen) combustion and gas flow dynamics of HVSFS process, modeling of secondary non-premixed (ethanol/oxygen) combustion, analysis of the interaction mechanism between gas and liquid droplet including fragmentation (secondary break-up), vaporization and finally analysis of the droplet injection point (axially, transversely, and externally), at the example of an industrial DJ2700 torch (Sulzer-Metco, Wohlen, Swizerland). In fact, this parametric study aims to explore the optimum parameters for HVSFS process and provide supplementary data to address the cooling effects observed by Dongmo et al. [22]. In addition useful conclusions are drawn from the analysis of different injection schemes previously unavailable in open literature. This study is based on and continues the numerical analysis of the conventional HVOF thermal spray process as described in author's earlier work [23,24].

Extensive validation of the combustion, discrete phase and flow model has been performed in earlier studies and therefore for brevity is not repeated here. The employed turbulent, combustion and spray models have been vigorously tested against experimental data, respectively, in the open literature and have demonstrated accurate predictions [23–27]. Thorough validation of the developed discrete phase break up sub-model employed in this study can be found in [27,28].

2. Model description

In the HVSFS system shown in Fig. 1 (HVOF torch was a Sulzer Metco DJ2700 Diamond Jet), premixed propane and oxygen are injected into the combustion chamber through annular inlet holes. The hot gas accelerates down through the nozzle which contains a convergent–divergent session. The coating material in the form of particles of size 30 to 200 nm, which is dispersed in organic solvent (ethanol), is injected into the main gas flow. The suspension spray then travels in the high temperature flow region, and its liquid part, evaporates and combusts along its trajectory. The remaining solid part of the spray which usually appears as fine agglomerates of nano-particles is accelerated and deposited on a substrate. The homogeneous liquid ethanol droplets are injected axially, transversely, and externally through an inlet as depicted in Fig. 1. For barrel and external positions, droplets are injected vertically. The working conditions for the simulation are summarized in Table 1.

The ethanol droplets after being injected into the HVSFS flame jet undergo several processes taking place simultaneously. The first is the aerodynamic break-up as the slow moving droplets are entrained into the high velocity jet and as they accelerate in the high velocity gas stream. Depending on their size and thermophysical properties of the liquid and the surrounding gas, droplets can undergo severe deformation and eventually break up into smaller droplets. To have a good understanding of the liquid spraying process, it is of fundamental importance to examine the physical break-up process instead of correlating the gas dynamics with droplet fragmentation indirectly. Although this study is intended to shed light on the importance of ethanol atomization process, the resulted droplet diameter distribution prior to injection are out of scope of this paper (primary break-up). The history of suspension droplets is computed with a Lagrangian formulation where the finite inter-phase transport rates and effects of turbulence interactions between the droplet and gas phases are considered. By using this treatment the evaporation history and temperature change for droplets can be calculated during the second process of heat exchange between the gaseous and liquid phases. The third process is the two phase combustion where ethanol vapors chemically react with the remaining oxygen from the primary propane-oxygen combustion. Finally, the subsequent gas flow pattern is detailed from the coupled set of equations described in the following section.

The conditions under which each droplet has a set of equations are:

1. The liquid droplet and oxygen gas phases have their own initial continuous velocity and temperature and co-exist at each location.
2. Liquid phase has its own turbulent fluctuations that result in turbulent droplet transport of mass, momentum and energy. The random effects of turbulence on the particle motion are counted by integrating the individual particle trajectory with the instantaneous fluid velocity.
3. The dissolved powder content is not included in this study and will be examined in a future paper. Although, the rate of evaporation and break of homogeneous ethanol spray might be different from the evaporation of suspension spray, it is assumed that the nano-particle loading is relatively low for this particular process.

The first part of model simulates the temperature and velocity fields of an HVSFS flame jet. The realizable k-ε model was used for modeling the turbulence in the jet, including compressibility effects. Both pre-mixed