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# Numerical investigation on effects of nanoparticles on liquid feedstock behavior in High Velocity Oxygen Fuel (HVOF) suspension spraying

Ebrahim Gozali [a], Mahrukh Mahrukh [b], Sai Gu [b,*], Spyros Kamnis [c,*]

[a] School of Engineering Sciences, University of Liverpool, Liverpool L69 3BX, UK
[b] Cranfield University, Cranfield, Bedford, Bedfordshire MK43 0AL, UK
[c] Monitor Coatings Limited, 2 Elm Road, North Shields Tyne & Wear, NE29 8SE, UK

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ABSTRACT

Suspension feedstock in high velocity oxy-fuel flame jets has opened a new area of research with great potential for advanced coatings. Understanding the suspension behavior in such a multidisciplinary process is a key factor in producing repeatable and controllable coatings. In this study, the effects of solid nanoparticles, suspended in liquid feedstock, on suspension fragmentation, vaporization rate and gas dynamics are investigated in the High Velocity Oxygen Fuel (HVOF) suspension spraying process by numerical modeling. 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. Moreover, the thermo-physical properties of suspension (mixture of solid nanoparticles and liquid solvent) are calculated from theoretical models. The results show that small droplets carrying high nanoparticle concentrations develop higher surface tension and result in less fragmentation. The recommended ethanol droplet size at high nanoparticle loadings is found to be 50 μm due to the high evaporation rate in the mid-section of the nozzle. For larger droplets, severe fragmentation occurs inside the combustion chamber (CC) while complete evaporation takes place in the free jet region outside the gun.



## 1. Introduction

High Velocity Oxygen Fuel (HVOF) suspension spraying is based on the conventional high velocity oxy-fuel (HVOF) thermal spraying process and was developed with the aim of spraying submicron or nanoparticle suspensions with hypersonic speed to deposit thin and very dense coatings [1–3]. HVOF suspension spraying uses a liquid solvent as a 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) [4]. Although a fairly wide variety of coating morphologies can be obtained, the size of microstructural features within the coatings is typically governed by that of the feedstock. Therefore, understanding liquid feed stock behavior in such a multidisciplinary system is important for its further development.

The HVOF suspension spraying process involves complex stages of droplet fragmentation, liquid droplet evaporation, nanoparticle agglomeration and nanoparticle/gas heat transfer coupling. The lack of experimental data and quantitative analyses of the internal regions of the torch makes modeling and numerical methods valuable tools for understanding the overall physics of the process by overcoming the technical constraints imposed by the experiments. Most importantly, in such a multidisciplinary process chemico-physical parameters are closely linked and make effective control of the process very challenging [5,6]. Composition of suspension feedstock, for example percentage of nanoparticles in the liquid solvent, is one of the most important parameters that affects the system outcome.

In the HVOF suspension spraying process the concentration of suspended solid nanoparticles in the solvent may vary from one case to another, depending on the application. The thermo-physical properties of suspension such as density, viscosity, specific heat, thermal conductivity and surface tension do not remain constant but differ according to nanoparticle concentration [7–13]. In addition, rate and final location of droplet evaporation in a thermal spray torch is critically governed by the physical properties of the solvent. This implies that assigning pure solvent properties or averaging solid and liquid properties in the suspension analysis may produce unrealistic results leading to a high level of errors in numerical simulations. This study will highlight this problem by providing a quantitative comparison between the vaporization rate of a typical homogeneous liquid solvent (ethanol) and non-homogeneous liquid suspension (ethanol carrying nanoparticles).

It must be noted that numerical analysis of the HVOF suspension spraying process has rarely been documented in the literature. Dongmo et al. [14] investigated the process by using the TopGun-G torch (GTV Verschleißschutz GmbH, Betzdorf, Germany). This modeling contains

* Corresponding authors.
*E-mail address:* Spyros@monitorcoatings.com (S. Kamnis).

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an overall discussion of the HVOF suspension spraying process in which both liquid ethanol droplets (300 μm) and solid titania particles (0.5–50 μm) are injected from the gun inlet with identical mass flow rates as discrete phases. The results showed that solid particles and liquid droplets moved with different velocities in the domain due to the differences in their properties. In another research study from this group, the combustion chamber of the gun was modified to a conical shape resulting in an increase in the process efficiency and avoiding nanoparticles contact with the combustion chamber walls [6]. However, in these studies the change in the liquid feedstock properties due to the nanoparticle inclusion was ignored.

The aim of this work is to analyze the influence of nanoparticle concentration and droplet diameter on the vaporization rate, the secondary breakup of the liquid phase, and the HVOF suspension spraying gas dynamics. The numerical analysis for this study consists of modeling pre-mixed (oxygen/propane) and non-premixed (oxygen/ethanol) combustions, interaction between gas and liquid phases (two-way coupling), secondary break-up and vaporization of droplets. Moreover, for modeling the suspension, the thermophysical properties are calculated from the theoretical models. This work is based on and continues the numerical analysis of the conventional HVOF thermal spray process as described in earlier studies [15,16]. Extensive validation of the combustion, discrete phase and flow model has been performed in earlier studies and therefore for brevity is not repeated here [15–19]. In addition, the details of validated discrete phase break up sub-models employed in this study can be found elsewhere [19,20]. Direct quantitative validation of the flow field within the gun is not possible with the current experimental equipment so the validation relies more on qualitative data.

## 2. Model description

The first part of the model simulates the temperature and velocity fields of the HVOF suspension spraying flame jet using the example of an industrial DJ2700 torch (Wohlen, Switzerland) as shown in Fig. 1. Working conditions for the simulations are summarized in Table 1 [21]. The Realizable k–ε model is applied here to simulate the gas phase turbulence and the gas flow is assumed to be compressible.

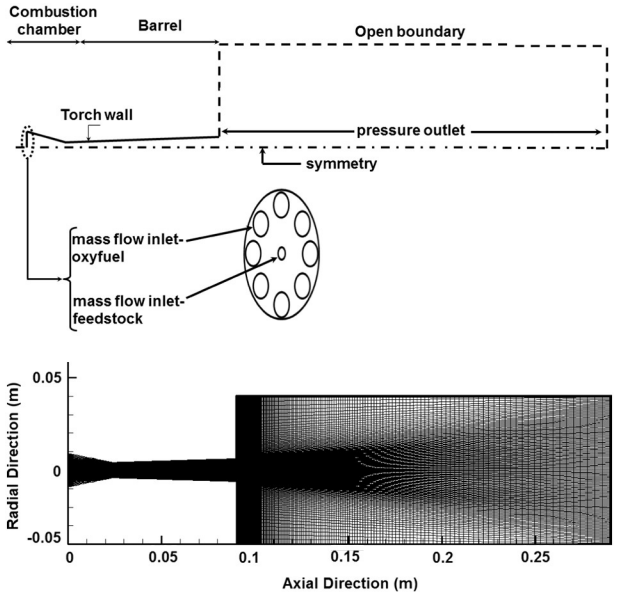


**Fig. 1.** Schematic diagram of the axisymmetric computational domain and boundary conditions.

**Table 1**
Operating parameters for the HVOF suspension spraying process.

| Working conditions | | |
|---|---|---|
| Propane | Flow rate: 0.003526 kg/s | Temperature: 300 K |
| Oxygen | Flow rate: 0.01197 kg/s | Temperature: 300 K |
| Atmosphere | Pressure: 101,325 Pa | Temperature: 300 K |
| Internal wall boundary | – | Temperature: 300 K |

Furthermore the eddy dissipation model is employed to model pre-mixed (oxygen/propane) combustion with hyper-stoichiometric oxygen mass fraction.

Discrete phase modeling (DPM) is used in this study to model the trajectory of the droplet/particle phase. The suspension properties undergo significant changes from the injection point to the landing location. The first stage is the aerodynamic break-up of droplets, as the slow moving droplets are entrained into the jet and accelerate in the high velocity gas stream. Depending on their size, the thermophysical properties of the liquid, and their interaction with the surrounding gas, droplets undergo severe deformation and then break up into smaller droplets. For the secondary breakup simulation, the Taylor Analogy Breakup (TAB) model is applied. The TAB model is suitable for droplets with low Weber numbers (We <100) and the model is, also, well adapted to the conditions of spraying and validated in earlier work [19]. A phase change will occur for liquid ethanol droplets after evaporation. Then the ethanol gas has to mix with excess oxygen, which remains after complete propane oxidation, due to molecular transport (diffusion) prior to reaction. Similar to the pre-mixed combustion, the eddy dissipation model is used to model this non-premixed combustion. The propane and oxygen flow rates indicated in Table 1 provide maximum flame temperature and velocity for DJ2700 torch (Sulzer-Metco) with hyper-stoichiometric oxygen mass fraction. For the HVOF suspension spraying, the oxygen mass fraction must be hyperstoichiometric in relation to complete ethanol combustion because the oxygen remnant will be used for ethanol combustion as diffusion flame. Mass flow rate of liquid ethanol droplets is 0.0001 kg/s, which is selected according to the results in the previous study [21]. The dissolved powder content is not included in this study and will be examined in a future paper instead the thermophysical properties of the suspension (mixture of liquid ethanol and titania powders) is calculated by theoretical models which in detail will be described in the following section.

Detailed descriptions of the gas phase, discrete phase, breakup, combustion models and droplet heat and mass transfer with continuous phase can be found elsewhere [15,16,19,21–24].

### 2.1. Effect of suspension

To model the suspension, the effect of nano-size particles on the liquid phase is considered as the change in the liquid bulk density, viscosity, specific heat, thermal conductivity, and surface tension. The density of suspension is defined as (Eq. (1)) [7]:

$$\rho_{susp} = (1-C)\rho_l + C\rho_p \quad (1)$$

where $C$ is the volume concentration of solid particles in suspension, $\rho_l$ is the density of liquid ethanol and $\rho_p$ is the density of solid titania — in this study the titania powders are considered to have a density of 4230 kg/m$^3$. Since the dissolved powder content is not charged into the suspension and instead its thermophysical properties are calculated by the theoretical models, discussing the type and size distribution of the nanoparticles are of less significance and it will be neglected in this work.

For modeling the viscosity of suspension, Einstein's formula is restricted for the low volume concentrations $\{\mu_{susp} = \mu(1 + 2.5C)\}$ and