Journal of Basic and Applied Engineering Research
Print ISSN: 2350-0077; Online ISSN: 2350-0255; Volume 2, Number 11; April-June, 2015 pp. 918-923

http://www.krishisanskriti.org/jbaer.html

Computational Study of High Velocity Oxygen Fuel Thermal Spray System

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Abstract—*High velocity oxygen fuel (HVOF) coating is a thermal spray coating process used to improve or restore a component's surface properties. It is typically used to deposit wear and corrosion resistant coatings on materials such as ceramic and metallic layers. A mixture of gaseous or liquid fuel and oxygen is fed into a combustion chamber, where they are ignited and combusted continuously. The fuel can be gases (methane, hydrogen, propane, propylene etc.) CFD technique can be used to closely simulate a thermal spray process and in- flight particle state during the spray process and can be calculated without actual experiments. In order to simulate combustion process different models such as, eddy dissipation, eddy dissipation concepts are used.*

Keywords*: Computational Fluid Dynamics (CFD); HVOF; Numerical Analysis; Thermal Spray Combustion.*

1. INTRODUCTION

Thermal Spray is an adaptable technology to produce protective coatings that enhance the performance of product that are coated through it. The thermal spray coating that uses the technologies have been developed into many derivates including the plasma, arc, flame, and high velocity oxygen fuel (HVOF) spray, that are based on the various methods of producing the energy. Thermal spraying also using the high velocity oxygen fuel (HVOF) process that is used to apply metallic, ceramic, and composite coatings to a variety of substrates in order to enhanced wear resistance, abrasion resistance, thermal and electrical insulation, and corrosion protection[1]. Better bond and mechanical strength are obtained by using HVOF spraying. The velocity of gas and particles are mainly higher in HVOF than those in plasma spraying achieved. The high velocities of particles is achieved by two factors, as first by HVOF torch normally generate supersonic external flows, but in plasma torches normally operate with a subsonic stream . Second factors in which the gas density in HVOF torches is mostly much higher than in the plasma torches, this event in this processes occurs because the gas peak temperature in the HVOF torches are much lower [2, 3]. In HVOF spraying the maximum temperature is about 3000K and in plasma spraying, it is approximately about 10,000K.The thermal spray using high velocity oxygen fuel (HVOF) is a coarse deposition process that consist the particles of micro size of metals, alloys or cermets that are propelled and heated in a sonic/ supersonic combusting stream of gas and are deposited on a substrate at high velocity to produce a thin layer of lamellar coating. HVOF thermal spray processes have been widely used in the automotive, aerospace, and chemical industries. For example WC/CO- based wear resistant coatings for drilling tools, and YSZ- based thermal barrier coatings for turbine blades and also Ni- based corrosion resistant coatings for chemical reactors [4]. The HVOF processes using different kinds of gun nozzle contours, such as convergent- barrel, convergent- divergent (or Laval nozzle), convergent multistage divergent and convergent divergent- barrel [5]. Without any nozzle the HVOF gun systems are also used. To improve the operation of the HVOF thermal spray process, a lot of experimental work has been done in the last decade for the study of the effect of operating parameters including gun type, fuel type, feedstock type and size, combustion pressure, fuel/ oxygen ratio and distance of spray on the particle temperature, velocity, melting ratio, oxidant content and the resulting coating macrostructure, porosity, hardness, wear abrasion and corrosion resistance [6-11]. In the study of HVOF systems the numerical modeling has a very important role, and also considered as specific tool for study of HVOF systems. The high velocity oxygen fuel (HVOF) thermal spray system has been also used in the aerospace industry for variety of surface coating applications for many years. Engineers of aerospace used the thermal spray coatings to insulating the various parts from heat, reduce turbine blade wear, and also protect against oxidation and corrosion. Diagram of the HVOF system, including combustion chamber, nozzle, barrel, particle injection, gas and particle flow field is shown in figure-1. The combustion of gases at high pressure and high temperature resulting from the combustion of oxygen and fuel expand through de Laval nozzle that is convergent and divergent in shape and the barrel to supersonic speed (local mach number M= 2). At the exit of nozzle the particle are injected into barrel. Particles are mixed turbulently, heated, and then accelerated inside the barrel. The physical and chemical condition of the particle that are striking on the substrate in turn is dependent on a large number of parameters such as gun design, particle size, shape, material, injection method. Powder particles with high speed gas jet, normally in the size range of 5-65µm. The field of coating processes and surface modification currently focus on the thermal spray coating of nanostructured through the concept of innovative technologies. This nanostructured also called the nanoscale, nanophase, and nanocrytalline materials in which the grain sizes are below 100 nm in the formal coating. Development of this technology is motivated by the discovery of properties of such materials that are superior to those of conventional bulk materials. The HVOF thermal spray process is very complex regarding the explanation in a theoretical model, because this process involves combustion, turbulence, compressible flow, multi components multiphase interactions, subsonic/supersonic transition, droplet deformation and solidification.

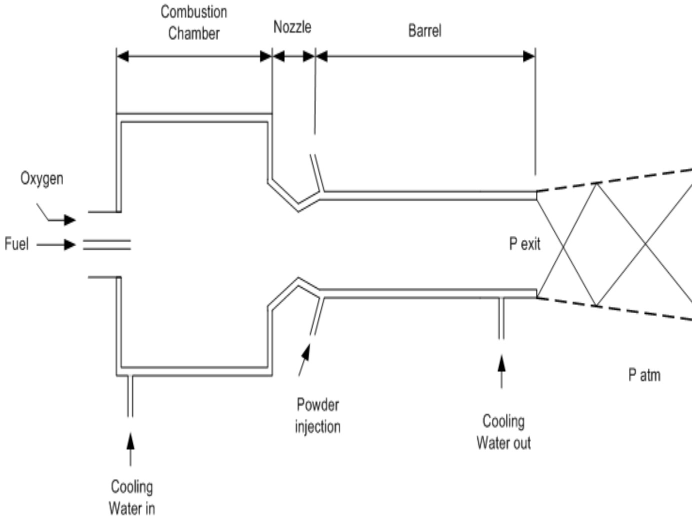

Fig. 1: Schematic of the high- pressure HVOF gun and flow field.

2. LITERATURE REVIEW

Kowalsky et al. investigated the flame spray Industries CDS torch through the various experimental processes. The torches that are investigated in various experiment uses the propylene and oxygen for combustion and a powder feed for particle injection. Velocities of alumina, tungsten carbide, and tribaloy particles in the torch plume were measured using laser two-focus velocimetry [5]. Measurements of pressure inside the torch and photo graphic measurements were made to determine various gas dynamic characteristics of the torch. Hackett et al. investigated the external gas dynamics of the Hobart-Tafa JP-5000, mainly free-jet mixing of the high temperature plume with the surrounding atmosphere [12]. Liquid kerosene fuel injection system used in this torch and it atomizes the fuel and reacts with gaseous oxygen [13]. Thorpe and Richter conducted the quantitative analysis of the gas dynamics and particle dynamics of HVOF spraying. Both the authors analyzed the internal and external flow of a newly designed HP/HVOF torch from Hobart TAFA Technologies, which is similar to the union carbide D- Gun [14-18]. They also calculated the energy release from an equilibrium chemistry model of heptane and oxygen, assuming no influence from the gas motion, and used one dimensional isentropic flow assumptions to compute the flow through a converging / diverging section of the nozzle. One dimensional flow assumptions were then used to compute the effect of friction (Fanno flow) in the constant diameter barrel of the torch. Outside the torch authors used the linerarized shock expansion theory to calculate the under expanded supersonic jet flow and also ignoring mixing with ambient air. Particle trajectories were also calculated, assuming no interaction with the gas stream. Analysis has used modern computational fluid dynamic (CFD) methods to simulate more complex physics in two dimensions. Some improvements in thermal spray modeling resulted from computational techniques developed for gas turbine engines and liquid and solid rocket motors. Literature presented axisymmetric, planar two dimensional and ionized flows, along the state of the art turbulence models. Researchers who have modeled thermal spray problems have used an Eulerian description of the gas flow, either an Eulerian or Lagrangian description of the dispersed phase. The affect of the particulate phase, that is either liquid or solid particles, on the continuous phase is taken into account by including interphase coupling terms in the equations. Some analyses have completely ignored the coupling of the particulate phase and the gas phase. The effect of the flow on the particles is computed by the simulations. In the Eulerian-Eulerian approach, sometimes referred to as the two fluid methods, a description similar to that of the continuous phase is also used for the particulate phase. In the Eulerian Lagrangian approach, a relatively small number of computational particles are used to model a large collection of physical particles, either solid or liquid. Ramshaw and Chang modeled thermal plasma using a two dimensional CFD approach with extensive plasma physics. The plasma was modeled as a multicomponent, chemically reacting gas in local thermodynamics equilibrium. Dissociation, Ionization, recombination, and other chemical reactions were computed by general kinetic equilibrium chemistry algorithms [19]. No particulates were included in the simulation. Chang also used a similar computational approach to model alumina spraying in an argon- helium plasma jet [20]. The representation of plasma is given as a continuous multicomponent, chemically reacting ideal gas with temperature dependent transport and thermodynamics properties. Lot of investigators have used CFD techniques to model the spray forming, or spray casting, process. EI-Haggar and Crowe also modeled the external two phase flow, including the stagnation of the flow on a flat substrate. They also used a PSI cell (practice- source-in cell) method and a finite difference method to solve the coupled two phase flow equations [21]. At nozzle exit the velocities were very small and temperature also relatively very low, therefore compressibility or chemistry is not considered. Berry et.al. Modeled the gas flow and liquid metal stream atomization inside a spray forming nozzle. Authors also considered injection of liquid metal from a slot at the throat of a converging diverging nozzle for planar two dimensional flows .They also used a density based formulation for the gas phase and an implicit, time iterative, finite difference method to solve the equations [22]. In this study by EI-Haggar and Crowe, the gas temperature and flow velocities were low, therefore no chemistry effects were considered and the flow was essentially incompressible. Power et.al. and smith et.al. Conducted the first CFD simulation of the HVOF spraying process. They also modeled both the internal and external flow of the metco diamond jet torch. In this, Powder is fed through a center tube using nitrogen as a carrier gas. Premixed oxygen and propylene are injected through an annulus in the nozzle. In this annulus the simplification of the eight small holes located circumferentially around the nozzle to introduce premixed fuel and oxygen. Air is injected in an outer annulus between the nozzle and the air cap to cool the air cap, since the torch has not any other cooling mechanism. The combusting subsonic flow was modeled inside the converging air cap, and the flow became choked at the exit of the air cap; that is it attained the sonic condition, external to the torch; they modeled the decay of the supersonic jet in a quiescent atmosphere. Because the pressure in the torch was greater than atmospheric pressure at the exit, the jet was under expanded. Their CFD simulation included a turbulence model for turbulent kinetic energy (k), dissipation rate (Ɛ) and combustion chemistry. The chemistry model included dissociation of the reaction products that used the two step, finite rate chemistry model and seven gas species: C3H6, O2, N2, H2O, CO2, CO, and H2 [23]. The finite difference equations, using a density based formulation were solved by an explicit time iterative scheme. Tracker particles of various sizes that responded to local gas velocity and temperature were injected inside the air cap near the centerline, but did not interact in any way with the gas stream. The analysis also did not account for any phase change of the particles [24]. D.Cheng et.al. Presented computed result of the given theory and describes the effects of operational parameters on the gas dynamics during HVOF thermal spraying. The mathematical model that has been implemented in this study allows for an appropriate representation of compressibility effects in the flow, combustion and turbulence. In this discussion authors take the maximum velocity of 2530 m/s and a maximum temperature of 3200K. Here the flame is expanded very slowly and cooled down rapidly through five repetitive expansion and compression waves that occurred after it exits the nozzle [25] S.Gu et.al. Showed a comprehensive CFD model, using CFX that has been developed to investigate the gas dynamic behavior in an HV2000 type HVOF thermal spray gun that is used the fuel gas propylene premixed with oxygen. The model was used to investigate the effects of the two different total gas flow rates and three levels of fuel to oxygen gas ratio on gas temperature, composition, and flow fields. The following conclusions have been obtained. In this process the centre temperature only reaches a value of 2500K. The gas velocity at the end of the nozzle is 1250m/s with a Mach number of one [26]. S. GU. et.al also explained the 2- dimensional axisymmetric CFD model, using CFX that has been developed to investigate the particle dynamic behavior in an HV2000 type HVOF spray gun using the fuel propylene premixed with oxygen. The model used a Lagrangian particle tracking frame coupled with a steady state gas flow field to examine particle motion and heating during HVOF spraying. The model was also used to investigate the effects of process parameters and chamber design on in flight particle behavior [27]. C.Bartuli et. al. explained computational modeling of the complex phenomena that take place in a high velocity oxygen kerosene spraying torch was approached by assuming simplified physical and chemical conditions for the combustion flame and for the solid particles in the torch and in the external field. Results of the simulation appear consistent with a number control parameters that were monitored during spraying, such as the power disperded for water cooling of the torch. The optimal Compromise for the material WC-Co composite particles that is represented by the use of an 8” barrel allowing particles velocities of 572m/s with a maximum temperature of 1568K, and by a spraying distance of about 200-300 mm from the final section of the barrel [28, 29]. S.Kamnis and S.Gu explained the numerical modeling of propane combustion in a velocity oxygen fuel thermal spray gun in which a CFD model had been developed to investigate the combustion and gas dynamics in an HVOF thermal spray gun using the liquid fuel propane. The global reaction model of propane combustion is able to give a reasonable prediction on heat generation, in term of flame temperature [30]. Hiroshi Katanoda et.al explained numerical simulation on supersonic flow in HVOF thermal spray gun in which internal flow of HVOF gun was analyzed that used a quasi one dimensional flow model in consideration of the effects of friction and cooling, and the supersonic jet from the gun was analyzed by using a numerical simulation of turbulent flow. From the computed results of the internal flow of HVOF gun and the supersonic jet from HVOF gun, the velocity and temperature of coating particles injected in the gun was calculated. In this analysis supersonic flow in the barrel of HVOF gun is greatly influenced by both friction and cooling [31]. V.R. Srivatsan and A. Dolatabadi explained simulation of particle shock interaction in a HVOF process in which the supersonic flow with particles strikes on three different substrates is simulated. Shock diamonds effects and bow shocks on the surface of the substrate on two different particle sizes namely 15 and 30 µm are analyzed. The particle of 15µm being very light are largely affected by the shock diamonds at the nozzle exit and bow shock near the substrate, whereas 30 µm particles are least affected by either shock diamonds or bow shocks. It will happen due to larger stokes number associated with 30 µm particles. The shape of the concave substrate is favorable for capturing all the particles. The strength of bow shock formed on a concave surface is very high that they deviated most of the lighter particles [13]. Mingheng Li and Panagiostis D. Christofides explained multi dimensional stochastic particle tacking model that explicitly accounts for turbulence in the gas phase and distribution of particle size and injection location. Velocity and temperature of particle are strongly dependent on particle size, although their spatial distribution on the substrate is minimal. The particle size distribution of the feed stock might be optimized to achieve desired particle velocity and temperature levels [4]. S.Kamnis and S. Gu also explained the three dimensional modeling of kerosene fuelled HVOF thermal spray gun in which three dimensional combustion flow within a kerosene fuelled HVOF thermal spray gun has been simulated using a commercial CFD code. The prediction from this numerical model can be summarized as the combustion process of Kerosene is dependent on the initial fuel droplet sizes. Small droplets generate a confined corn shape flame and give more uniform temperature profile within the combustion chamber while large droplets have dispersed fan shape flame structure and less uniform temperature profile. Possibility to overcome the problem of carbon deposition from the current design by changing the incoming angle of fuel and oxygen stream towards the centre will effectively reduce the contact between the combusting gas and the internal wall surfaces [32]. Hiroshi Katanoda analyzed the effects of the pipe friction cooling and nozzle geometry on gas and particle flow in HVOF thermal spray gun. In which author give the concept of effects of pipe friction, cooling and nozzle geometry on the particle behavior as well as supersonic gas flow in the HVOF gun that were investigated by using the quasi one dimensional analysis and nozzle, a 7.9 mm throat diameter and 11 mm exit diameter. And length of nozzle also varied in the range of 110-330 mm [33]. N. Zeoli et.al. Also explained the numerical simulation of in fight particle oxidation during thermal spray and analyzed an oxidation model has been implement in Lagrangian method for tracking powder particles in thermal spraying. Numerical models are used for parametric study on particles size and injection location. The given investigation has used stainless steel powders, but the oxidation model can be generically applied to any metallic powders in thermal spray coating [1]. E. Dongmoet.al. had given the analysis and optimization of the HVOF process by combined experimental and numerical approaches in which they concentrated on the three modeling and simulation approach to HVOF thermal spray processes based on an Euler-Lagrangian formulation and applied to the Processing of alumina particles using the fuel gas propane. The industrial HVOF Top Gun –G torch design was modeled and the two phase supersonic, turbulent and reacting flow with under expanded fluid conditions at exit of the nozzle was solved using the commercial CFD program ANSYS CFX. Temperature of the particle and velocity of particle play an important role in the formation of coating microstructure. Modeling approaches fluid structure coupling for analysis of coating formation and the influence of the impinging gas jet on the substrate will be considered [12]. S. Hossainpur and A.R. Binesh focused on a CFD study of sensitive parameters effects on the combustion in a high velocity oxygen fuel thermal spray gun and here authors focused on gas dynamics features that exist inside and outside a high velocity oxygen fuel (HVOF) thermal spray gun in which premixed oxygen and propane are burnt in a combustion chamber linked to a parallel sided nozzle. The velocity of gas, temperature, pressure and Mach number distributions are presented for various locations inside and outside the HVOF system. The two dimensional numerical simulations showed large variations in gas velocity and temperature both inside and outside the torch to flow features such as mixing layers, shock waves and expansion waves. Here the maximum gas temperature only reaches 3300K close to the annular flame front, the centerline temperature only reaches a value of 3000K and velocity of end of the nozzle is about 2500 m/s and has a mach number of 2.3[34]. L. Ajdelsztajn et.al. Also focused on a comprehensive CFD model based on CFD-ACE that had been applied to investigate the gas flow behavior in a specific HVOF thermal spray system. Here the model was used to investigate the influence of three different fuel to oxygen mass ratios on gas temperature and velocity distributions and their effects on particle temperatures and velocities of Fe-based amorphous glass during spraying. Here numerical results obtained with the particle thermal model were compared with those obtained in a simpler model and have good degree of agreement for the operating conditions considered in this work [35]. H. Tabbara and S.Gu also explained the concept of Computational simulation of liquid fuelled HVOF thermal spraying in which they explained the theory of premixed steady state flame and compressible combustion flow that had been simulated within a kerosene fuelled HVOF thermal spray gun that used the commercial CFD fluent 6.3[36].

3. MATHEMATICAL MODELS

Gas flow model

The equations that are governing the three dimensional model in the Cartesian tensor form are:

Mass conservation equations

$$\frac{\partial p}{\partial t}+\frac{\partial}{\partial x_i}(\rho\mu_i)=0 \tag{1}$$

Momentum conservation:

$$\frac{\partial}{\partial t}(\rho\mu_i)+\frac{\partial}{\partial x_j}(\rho\mu_i\mu_i)=-\frac{\partial p}{\partial x_i}+\frac{\partial}{\partial x_j}\tau_{ij}+\rho g_i \tag{2}$$

Energy transport equation

$$\rho\frac{\partial T}{\partial t}+\rho\mu_i\frac{\partial T}{\partial x_i}=\frac{\partial}{\partial x_j}(k\frac{\partial T}{\partial x_j}+\tau_{ij}\mu_i)+\rho g_i\mu_i+q_h \tag{3}$$

Where the stress tensor is given by

$$\tau_{ij}=\mu(\frac{\partial u_j}{\partial x_i}+\frac{\partial u_i}{\partial x_j})-\frac{2}{3}\mu\frac{\partial u_i}{\partial x_i}\delta_{ij} \tag{4}$$

Particle model

Equations of motion: The equation of motion that used for particles can be written as a force balance that equates the droplet of the inertia with forces acting on the droplet,

$$\frac{du_p}{dt} = F_D(u - u_p) + \frac{g_x(\rho_p - \rho)}{\rho_p} + F_x \tag{5}$$

The drag force per unit particle mass is

$$F_D = \frac{18\mu}{\rho_p d_p 2} \frac{C_D R_e}{24} \tag{6}$$

The drag coefficient C_D given by morsi and Alexander (1972)

$$C_D = \frac{24}{\mathrm{Re}_d}(1 + b_1 \mathrm{Re}_d{}^{b2}) + \frac{b_3 \mathrm{Re}_d}{b_4 + \mathrm{Re}_d} \tag{7}$$

$$\begin{aligned} b_1 &= \exp(2.3288 - 6.4581\phi + 2.4486\phi^2), \\ b_2 &= 0.0964 + 0.5565\phi, \\ b_3 &= \exp(4.905 - 13.8944\phi + 18.4222\phi^2 - 10.2599\phi^3), \\ b_4 &= \exp(1.4681 + 12.2584\phi - 20.7322\phi^2 + 15.8855\phi^3) \end{aligned} \tag{8}$$

The shape factor ϕ given by Haider and Levenspiel (1989) is

$$\phi = \frac{s}{S} \tag{9}$$

The relative Reynolds number is defined as

$$\mathrm{Re} = \frac{\rho d_p \,|u_p - u}{\mu} \tag{10}$$

Turbulent model

A wide variety of flow problems can be calculated by using the standard k-Ɛ model (Launder and Spalding, 1972) based on the presumption that an analogy between the action of viscous stresses and Reynolds stresses on the mean flow exists. The transport equations for the realizable k-Ɛ model are

Turbulent kinetic transport equation:

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho k u_j) = \frac{\partial}{\partial x_i}\left[\left(\mu + \frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right] + G_k + G_b - \rho\varepsilon - Y_M + S_k \tag{11}$$

Rate of dissipation of energy from the turbulent flow:

$$\frac{\partial}{\partial t}(\rho\varepsilon) + \frac{\partial}{\partial x_j}(\rho\varepsilon u_j) = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_j}\right] + \rho C_1 S\varepsilon - \rho C_2 \frac{\varepsilon^2}{k + \sqrt{\upsilon\varepsilon}} + C_{1\varepsilon}\frac{\varepsilon}{k}C_{2\varepsilon}G_b + S_\varepsilon \tag{12}$$

Where the turbulent viscosity is

$$\mu_t = \rho C_\mu \frac{k^2}{\varepsilon} \tag{13}$$

The coefficient of dynamic viscosity is

$$C_\mu = \frac{1}{A_0 + A_s(kU/\varepsilon)} \tag{14}$$

In the comparison with the standard k-Ɛ model, the realizable k-Ɛ model contains a new formulation of the turbulent viscosity where the dynamic viscosity coefficient is no longer constant (Shih et. al. 1995).

4. CONCLUSIONS

The velocity and temperature of particles shows a important role in the formation of the coating microstructure especially in the fabricating nanostructured coatings. It is very crucial to maintain high particle temperature and velocity as well as gas pressure at the point of impact on the substrate, but also to prevent particles from being superheated. Friction in pipe has a larger effect on the gas /particle velocity. In other words we can say that the cooling has a larger effect on the gas/particle friction causing a decrease in gas particle temperature. The velocity and temperature of particles are strongly dependent on particle size, although their spatial distribution on the substrate is minimal. Particle size distribution of the feed stock might be optimized to achieve desired particle velocity and temperature levels. Numerical simulation of two dimensional presented large variations in gas velocity and temperature both inside and outside the torch due to flow features. Mixing layers, shock waves, and expansion waves are the example of the analysis of the two dimensional numerical simulation.

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