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Three-dimensional numerical simulations of the particle loading effect on gas flow features for low pressure cold spray applications

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ABSTRACT

This paper reports numerical investigations to develop a high quality simulation model for the Cold Spray (CS) process as part of the project, Supersonic Spray Advanced Modelling (SSAM). Cold spray is a process in which unmelted solid particles are accelerated through a De Laval nozzle toward a target surface and deposited, which avoids or minimises the detrimental effects that arise from melting. The gas flow injected allows the particles to achieve velocities up to 1000 m/s until they impact onto a substrate, bonding with plastic deformation. Analytical and numerical tools were used in the recent years to study the most important parameters of the fluid dynamic of the process. These parameters are often overestimated or non-validated, as many authors tend to neglect inter-phase couplings. The interactions between the gas flow features and particulate phase are important for the present multiphase flows, and many of the connected phenomena lack physical comprehension. For this purpose, a detailed 3D model for RANS simulations has been realised and the gas and particle dynamics in the nozzle and jet were analysed. Advancements for future computational methods are derived from this study, in order to build a comprehensive and coherent numerical model for cold spray applications.

1. Introduction

Cold Spray (CS) is a relatively recently developed coating technology, in which a feedstock material in the form of powder is accelerated by a process gas in a converging-diverging nozzle and impacted onto a substrate. In order to achieve particle-substrate bonding, particles require a material-dependent minimum impact velocity, called the critical velocity [1]. The process makes use of the high kinetic energy rather than thermal energy (unlike traditional coating technologies), which allows for a low temperature deposition process. No melting is therefore involved in the process, so that detrimental effects such as oxidation, crystallization, gas releases, high residual stresses and other thermal effects are widely eliminated or minimised [2,3]. It also leads to the advantageous possibility to form coatings of composites, e.g. reinforced with diamonds, which could not be deposited otherwise [4]. Experimental and numerical studies on the two-phase nozzle flow were conducted in the past decades, identifying the main parameters for gas and particle acceleration: the gas stagnation pressure and temperature [5,6], the gas species [7,8] and the powder injection conditions [9,10]. Other crucial aspects are the particle size, morphology and material, as the larger and heavier particles are the less susceptible to the flow, having a much higher characteristic reaction time [11–13]. Possible particle shape irregularities are connected to the drag coefficient [14,15].

Because the most important fluid dynamics takes place within the nozzle, where it cannot directly be observed, the design and analysis of the process strongly depend on computational methods. Since the micron-sized particles are transported through a gas phase, which reaches a supersonic regime, models required to be greatly simplified in the past. However, the current availability of computer power, allows for computational fluid dynamics (CFD) to predict the above-mentioned properties in more detail. Some authors [16,17] have provided an overview of the most common numerical methods used to investigate the coupled flow parameters and understand the bonding mechanism. Both publications have pointed out the convenience of using numerics to predict the fluid dynamics of the cold spray process in comparison with experimental measurements. The validity of the models is strongly case-dependent and in most cases, the two-way exchange of energy and momentum between phases is ignored on the assumption of very low particle loading. However, results on this parameter are rare and ambiguous. Samareh et al. [18] indicated that particle speed reduces as particle mass fraction increases, and that this induces significant changes in gas flow structures. Accordingly, a study by Lupoi [19] showed that experimental nozzle performance analysis could not be explained by a standard one-way coupling CFD technique. When increasing the detail of phase coupling for such experiments, the trends

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could be improved [20]. Faster processing within CS manufacturing demands for higher feed rates, with a more realistic understanding of the gas-particle mixture behaviour that has commercial benefits [21]. Recent works identifying driving mechanisms for losses and comparing different materials in this respect, both experimentally and numerically [20], [22], find that the two-dimensional computations involving a two-way coupling can capture velocity trends, but fail to quantitatively predict particle behaviour. A more detailed analysis of this mechanism and the construction of a more holistic numerical model are therefore required.

The first three-dimensional(3D) numerical model was developed by Han et al. [5], reporting that simulations based on CS applications are possible. However, this work was conceived to be for initial parameter studies. Soon after, Karimi et al. [23] led numerical simulations of a very specific case, involving an oval nozzle without phase coupling, whose velocity validation required further modification. Tabbara et al. [24] conducted 3D numerical simulations on particle dispersion of different size in the jet, using nozzles with different cross sections. However, the one-way coupling model didn't take into account the loading effect, nevertheless results showed similar trends with compared experimental values. Other works conducted by Yin et al. [25] and Zahiri et al. [26] were addressed to outline the 3D simulations as an efficient method to approximate process variables for the gas phase, although they ignored the two-way coupling in the analysis. The latter work was used as starting point by Faizan et al. [27], which developed one of the most detailed 3D existing model.

This study aims to provide a computational model for a low stagnation pressure CS nozzle. It focuses on the model development and details the interplay of physical aspects. Herein, the velocity is most important, being the crucial quantity in the process. Besides this, the coupled fluid mechanics are explained by thermal and turbulence analysis.

The reasons for which low pressure was chosen to be studied in the present paper are related to the initial design phase of an experimental rig, which is aimed to perform Particle Image Velocimetry (PIV) on nozzle-internal particle flow, which dictates the physical dimensions. The requirement to study the fluid dynamics inside the duct with such technology emerges from the direct observation of the nozzle-internal mechanisms. The numerical methods employed in this work were previously validated initially through measurements of the particle speed in the jet using a similar apparatus (reference as in reviewer response). Since both mass and volume of particles seem to play a role, the actual interactions within the nozzle are required to be observed, in order to provide validation for the aspect under consideration. Such a study is viewed as follow-up work that should focus on the details of such experimental observations. In order to underline the present observations nonetheless, they are compared against a conventional and a coupled two-dimensional model, substantiating the importance of model detail. The nozzle is a particular in-house design for a new measurement approach and present computations are used to optimise the nozzle for such future experimental studies. The goal of this study is the assessment of the adequacy of computational methods that are widely used in the field of CS and how they can be amended with limited effort to obtain models of higher validity.

2. Governing equations and framework

Being the most commonly used package in the field of CS simulations, the commercial CFD software ANSYS®FLUENT is employed in this study. The particulate phase is not spatially interconnected, while the gaseous component such as air, nitrogen or helium is continuous. The disperse and the continuous phases are hence described by two different sets of equations. In some cases, the extended and coupled version of the conservation laws is used, called the Eulerian-Lagrangian framework, details of which are described in this section.

2.1. Gas phase equations

The physics of the continuum phase is described by the conservation of the mass, the momentum balance equation and the energy balance equations. These principles result in a set of coupled, hyperbolic-parabolic partial differential equations known as Navier-Stokes equation, which is the most general description of fluid mechanics [28]. The common approach is to consider a time- or ensemble-averaging process, which yields to the well-known Reynolds-averaged Navier-Stokes equations (RANS). For the closure of the Reynolds-averaged equations, additional expressions for the Reynolds-stresses are required, and two approaches can be distinguished. The first is used for Reynolds Stress Models (RSM), where all turbulence-induced stress components are modelled separately. Due to high computational effort, the second approach, the concept of Eddy Viscosity Models (EVM), is used here. The present simulations employ the realizable k-ϵ model for the eddy viscosity, solving additional transport equations for the turbulent kinetic energy k and dissipation rate ϵ. Models often used in CS like the standard or the re-normalization group (RNG) k-ϵ model, have weaknesses in dissipation rate modelling, which can cause poor performance in highly dissipative flows such as axisymmetric jets [17]. In the realizable k-ϵ model the transport equation for the dissipation rate is derived by imposing a realistic condition of non-negativity on the mean-square vorticity fluctuation, providing superior performance for flows involving boundary layers under strong adverse pressure gradients. In a CS flow, this is relevant mostly in the nozzle exit and free jet region. The RANS and turbulence model equations are well known and can be studied in detail elsewhere.

2.2. Lagrangian particle tracking

In the Eulerian-Lagrangian framework, the particles are solved in a Lagrangian reference frame, which moves with the particles, and is connected through coupling laws to the gas phase that is solved in the Eulerian frame. This way, the motion of a particle can be integrated simply along its trajectory using a force balance. Particles do not have physical volume but are represented as point masses, which impose a restriction to relatively low volume fractions (< 12%) on the discrete phase. For the equations of motion, we need to define particle Reynolds and Mach numbers for the relative flow of gas around particles: $Re_p = \rho_c D_p |u_c - u_p|/\mu_c$, $Ma_p = |u_c - u_p|/\sqrt{\gamma R T_c}$. Variables are referred with index c and p for the gas and particles respectively. The momentum conservation law for a single particle per unit mass can then be expressed as:

$$\frac{d\vec{u}_p}{dt} = \vec{F}_p(\vec{u}_c - \vec{u}_p) + \frac{\vec{g}(\rho_p - \rho_c)}{\rho_p} + \vec{F} \tag{1}$$

$$F_D = \frac{18\mu}{\rho_p D_p^2} \cdot \frac{C_D Re_p}{24} \tag{2}$$

where the gravitational term is dropped and the drag coefficient c_D needs to be modelled. In literature, the standard law is defined by Morsi and Alexander [29], which determines the drag coefficient for a spherical particle for a wide range of particle Reynolds numbers. However, this law does not take into account compressibility effects, which are primary in cold spray. Therefore, it is more advisable to use the Henderson-law [30], which is subdivided into three Mach number ranges for subsonic, transonic and supersonic relative flow, or, as in this study, the law proposed by Clift et al. [31]. It is applicable to moderate relative Mach numbers of larger than 0.4, limited by maximum relative Reynolds numbers of 300,000. It is worth noting that the validity of these drag models in CS simulations is still a matter of discussion [17].

Local velocity fluctuations have a significant impact on the particle motion and can affect particle trajectories. A turbulent dispersion for particles through a stochastic tracking (random walk) has been used to