Computers & Fluids 113 (2015) 32–41

Contents lists available at ScienceDirect

Computers & Fluids

journal homepage: www.elsevier.com/locate/compfluid

Penalty and Eulerian–Lagrangian VOF methods for impact and solidification of metal droplets plasma spray process

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ARTICLE INFO

Article history:
Received 12 March 2014
Received in revised form 22 September 2014
Accepted 8 October 2014
Available online 4 November 2014

Keywords:
Multi-phase flow
VOF
Eulerian/Lagrangian approach
Heat transfer
Phase change
Thermal contact resistance
Spreading and plasma spray

ABSTRACT

The direct numerical simulation of the impact and solidification of a tin droplet on a solid substrate is investigated by means of a volume of fluid sub-mesh method Vincent et al. (2010), which is extended for the first time to the solving of the energy equation with phase change. In addition, viscous penalty methods are proposed to treat the solidifying part of the droplet as it spreads onto the target substrate. The presence of a thermal contact resistance is also tackled within the proposed model. The numerical modeling is validated against various typical configurations of phase change with interface that provide analytical solutions. Among them, we can cite the contact of two materials with a thermal contact resistance or the Stefan problem for the propagation of a solidification front. The last part of the article is devoted to the numerical simulation of the impact of a tin droplet on a flat substrate. The simulations are compared to experiments of Aziz and Chandra (2000) and a study on the value of the thermal contact resistance is proposed.

1. Introduction

Plasma spray process (PSP) is one possible way to heat, to melt and to deposit ceramic or metallic micrometer size particles which are injected in a plasma flame as a power jet [3,4]. At the last stage of powder spreading by PSP, the particles impact onto a chosen substrate in order to build a thin coating. PSP is currently used to deposit functionalized thin coatings onto mechanical devices and to manufacture for example thermal barriers or chemically neutral material surfaces. The mechanical and thermal properties of the thin boundary coating (TBC) are directly resulting from the quality and the type of droplet impact on the target substrate, as explained for example in [4,5]. Thermal and velocity conditions encountered in the plasma flow make experimental coating observations difficult to investigate. In particular, time history of droplet impact, spreading and solidification is almost impossible to observe and to characterize [6] except for a single snapshot. The available measurements for micrometer size particles are describing the final properties of the resulting TBC at only a macroscopic scale after impact and solidification of all droplets and particles. The final shape of the particles are sometimes captured instantaneously however without any description of their time evolution. The only recent plasma spreading experiments of impacting particles that attempt to describe the time evolution of the particle shapes during impact concern millimeter size particles [7]. Understanding how the micrometer size molten particles spread, deform and solidify is still a scientific challenge that can only be addressed by a complete numerical simulation at small scale of the mass, momentum and energy conservation [8]. It is of major importance to characterize the generation of pores inside the structures and the quality of the resulting TBC. This is the subject of the present work.

Our main objective is to propose a physical model and numerical methods in order to describe the small scale interface deformations and shapes during ceramic or metallic droplet impact with solidification during TBC manufacturing. Small scale numerical simulations have to be able to handle for droplet/gas interface transport and deformation while solving at the same time, solidification, thermal contact resistance, capillary and wetting effects. For characterizing the deposition of metallic particles on a substrate, physical phenomena appearing during the process are various: turbulence, compressibility, surface tension, wettability, heat transfer and phase change. Specific models and a computational fluid dynamic (CFD) code have been developed and validated to integrate these various phenomena into a numerical modeling for plasma flow

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http://dx.doi.org/10.1016/j.compfluid.2014.10.004
0045-7930/

and ceramic droplet impact on a substrate. Among the wide literature devoted to PSP, no local simulation of droplet impact can be reported, due to the complexity and non linear character of the physical processes and also to the difficulty of handling at the same time gas/particle and liquid/solid deformable interfaces during impact and solidification. The majority of existing works concerning the modeling and simulation of heated particles in PSP flows concern the Lagrangian description of the thermal and size histories of powders and particles inside the plasma flame before impact on the target substrate [9] or for nanometer size suspension plasma spraying conditions [10–12]. Only one research group [13–15] reports on the local and instantaneous description of impact and solidification of a particle onto a substrate under plasma conditions and it concerns millimeter size particles. In these publications, both experimental views and simulations coming from an interface tracking approach on fixed grids are illustrated. The numerical methods described below belongs to the same class of volume of fluid modeling and numerical methods as in [13–15], but our approach is different in many points: our model is compressible, we use fictitious domains methods to account for solid media and our numerical schemes for solving interfacial quantities (liquid and solid fraction inside the particles, temperature) are Lagrangian and not Eulerian.

Based upon our experience in simulating compressible non-isothermal multi-phase flows at small scale, we propose to adapt our models and numerical methods to the impact and solidification of micrometer size droplet under PSP conditions. Those models are based on a compressible augmented Lagrangian like formulation of the mass and momentum conservation equations [16–18], large eddy simulation modeling for turbulence [19–22] and implicit interface curvature estimate for the surface tension and wetting effects [23]. By implicit interface curvature, it must be understood that no explicit geometric information on the interface position or topology is used, only the presence VOF function is utilized through its gradient. These models are coupled to a fictitious domain description of the multi-material flow (plasma medium, ambient air, liquid and solid particle phases and also substrate) which uses characteristic volume of fluid (VOF) functions on a fixed Cartesian grid. The properties of all media (gas, liquid or solid) are imposed in an implicit way by penalty techniques [24–27]. The model and numerical methods are described in detail in Section 2. Section 3 is devoted to presenting a multi-scale VOF-SM method which has been extended to heat transfer and solidification [1]. The numerical model is validated against experiments of Pasandideh-Fard et al. [28] for the single impact and solidification of a millimeter size metallic droplet. Conclusion and perspectives are finally drawn.

2. Model and general numerical methods

Describing the small scale heat transfer and flow motion during the impact and solidification of one or several droplets on a substrate requires being able to investigate the deformation of various interfaces between several phases such as plasma, liquid and solid parts of the impacting particle as well as substrate surface. A typical configuration is illustrated in Fig. 1. Three types of interfaces have to be tracked during time: a standing surface between the target substrate and the rest of the multi-phase flow, the particle phase interface during impact, spreading and solidification and the solidification interface inside the particle. The two last interfaces are not know *a priori* and result from the thermal and motion coupling between the interaction of the plasma, the particle and the substrate. Using deformable grids to handle interface tracking is a very difficult task in three dimensions [29] as a remeshing is required at each time step due to interface deformation. We choose to use fixed Cartesian grids not adapted to the topology of interfaces in order to model the multi-material flow of impinging droplets with solidification. The presence of interfaces will be tackled with characteristic functions and penalty methods, as explained in the following sections.

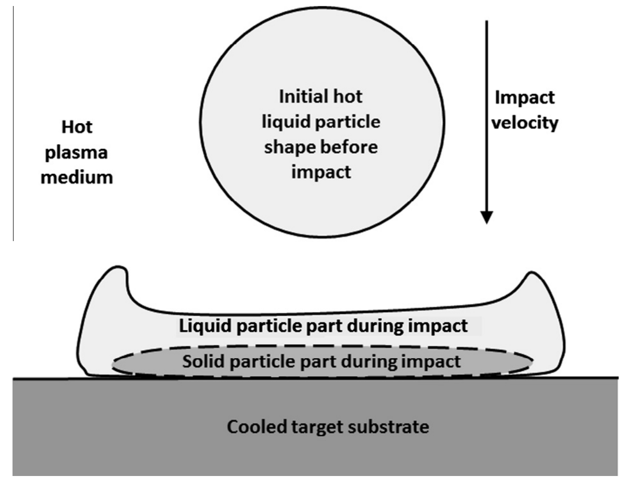

Fig. 1. Typical multi-material topology during the impact and solidification of a droplet in a PSP process.

2.1. Multi-phase modeling of droplet impact with solidification

Multi-phase flows involving a carrier fluid and a liquid or a solid phase can be modeled by solving the compressible Navier–Stokes equations [16] together with a phase function C describing the particle phase shape evolutions through an advection equation on the corresponding phase function. By definition, C is equal to 1 in the phase to be located and 0 elsewhere. In our problem, a characteristic function for the droplet phase is defined as C_d, which is equal to 1 inside the particle and 0 in other media. We also use C_{sd} the characteristic function for the solidified part of the particle, which is equal to 1 in the solid particle zones and 0 elsewhere. By definition, C_{sd} can be equal to 1 only if C_d is equal to 1. The last characteristic function introduced is C_s for the substrate, being equal to 1 in its interior and 0 in the fluid and solidified particle parts of the flow. By definition, if $C_s = 0$ and $C_d = 0$, we are inside the mixture of air and plasma fluid.

As explained by Kataoka [30,31,16], a resulting one-fluid model can be built that implicitly takes into account the jump relations at the interface [32,33] including surface tension effects and also manages the fluid–fluid or fluid–solid interface evolutions in an Eulerian manner by solving additional advection equations on the characteristic functions as follows:

$$p^{new} = p^{old} - \frac{\tau}{\chi_T}\nabla\cdot\mathbf{u} \tag{1}$$

$$\rho\left(\frac{\partial\mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u}\right) - \frac{\mu}{K}\mathbf{u} = -\nabla\left(p^{old} - \frac{\tau}{\chi_T}\nabla\cdot\mathbf{u}\right) + \rho\mathbf{g} + \nabla\cdot\left([\mu+\mu_t](\nabla\mathbf{u} + \nabla^t\mathbf{u})\right) + \mathbf{F}_{st} \tag{2}$$

$$\rho c_p\left(\frac{\partial T}{\partial t} + \mathbf{u}\cdot\nabla T\right) = \nabla\cdot[(\lambda+\lambda_t)\nabla T] + \rho L\frac{\partial C_{sd}}{\partial t} \tag{3}$$

$$\frac{\partial C_d}{\partial t} + \mathbf{u}\cdot\nabla C_d = 0 \tag{4}$$

$$\rho = C_s\rho_s + (1-C_s)C_d\rho_d + (1-C_s)(1-C_d)\rho_g(p,T) \tag{5}$$

$$\mu = C_s\mu_s + (1-C_s)(1-C_{sd})\left(\frac{\mu_d\mu_g(p,T)}{C_d\mu_g(p,T) + (1-C_d)\mu_d}\right) + C_{sd}\mu_{sd} \tag{6}$$

$$\lambda = C_s\lambda_s + (1-C_s)\left(\frac{\lambda_d\lambda_g(p,T)}{C_d\lambda_g(p,T) + (1-C_d)\lambda_d}\right) \tag{7}$$