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# Numerical simulation of several impacting ceramic droplets with liquid/solid phase change

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ABSTRACT

This paper is dedicated to numerical simulations of impact and solidification of several ceramic droplets on a solid substrate. This process is usually encountered in ceramic plasma spraying to manufacture thick coatings. The characteristics of the final product are deeply related to the impact conditions of the droplets, since the particles can interact with the substrate or with neighboring droplets and induce a variable porosity. The objective of the numerical simulation is to gain a better understanding of the coating properties during its elaboration. This paper describes the numerical code based on a finite volume discretization, and presents the results of successive droplets impacting, in terms of hydrodynamics, thermal flux and solid fraction evolutions with time for one given configuration.



## 1. Introduction

Plasma spraying is a well-known process for manufacturing thin or thick coatings. This technology is often used to obtain high-performance material characteristics, like insulation and hardness, on industrial parts with complex shapes. The fluid particles (typical diameter of D = 30 μm) impact the substrate with a typical velocity of 150 m $s^{-1}$, in a molten or semi-molten state [1,2]. Under such conditions, the fluid dynamics may result in a splat or splashing phenomenon, depending on several parameters such as the temperatures of the substrate and particle. The first droplets collide with the substrate that is assumed to be plane, whereas the following ones reach a surface made of previously spread droplets, with an inhomogeneous surface topology. The potential behavior is widely dependent on the state of the droplets, as an impact on previous droplets having solidified completely does not render the same dynamic and thermal evolutions as an impact on a partially or totally liquid surface. Theoretical and experimental analyses can be found in the literature [3–5] concerning the behavior of single droplets. Some numerical studies have been carried out to understand the particles behavior. For example, Zhang et al. [6] have proposed a smoothed particle hydrodynamics method to simulate the impact and solidification of a single yttria-stabilized zirconia droplet onto an inclined substrate at high velocity. Their results revealed the influence of the surface tension on the dynamic. They found that splashing occurred for a critical impact angle of approximately 44°. Pasandideh-Fard et al. [7] provided a numerical presentation of how a single metal droplet behaves while impacting horizontal or inclined substrates, using a finite element method on a 3D Cartesian grid. They took into account solidification and a thermal contact resistance, and demonstrated that the hydrodynamic and thermal behaviors were close to the experimental counterparts.

Concerning interactions between several droplets, Haferl and Poulikakos [8] investigated the experimental deposition of successive droplets at the same position at low velocity. They have obtained a pile-up where the spreading factor remains low. The spreading is linked to the substrate temperature and the shape of the previous flattened droplets. Ghafouri-Azar et al. [9] explored the impact and solidification of two droplets one on the other with an offset of impact position. Their numerical results were compared to experiments, and the spreading was found to be more effective on the smooth substrate than on the previous droplet. More recently, a simple numerical approach was proposed by Le Bot and Arquis [10] to estimate the heat flux time evolution for successive layers impacting a substrate, without dynamics and the results show that for a high impact frequency, remelting can partially occur before total solidification. Wang et al. [11] used numerical simulation to investigate the behavior of the solidification front of several deposited droplets, assuming that they all gave rise to a splat shape. The substrate was made of the same material as the splats, and that total solidification was completed prior a new splat impact. Their results revealed that temperatures, thermal contact resistance, splat thickness and impact frequencies could induce a partial remelting of the material. Le Bot et al. [12] performed another numerical simulation with a finite volume method on a 2D Cartesian domain to study the presence of air traps during impact and solidification of indium droplets and found that a rapid solidification tended to retain air bubbles, whereas the bubbles could be ejected if hydrodynamics were preponderant upon solidification.

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The objective of the present article is to numerically describe the thermal behavior of several droplets impacting a substrate under plasma spraying conditions, taking into account the solidification. One configuration is proposed, with given droplet and substrate temperatures, with constant properties, and the corresponding phenomena are described and commented. It is the first step of a wider study of the plasma spray process from the plasma jet to the coating manufacturing from droplets impact, with a Eulerian point of view. The originality of this work is based on the micrometer scale used for the multiple impacts. First, the physical model is described, followed by the numerical methods to solve the dynamics, and a presentation of the thermal field and the solidification progression. Finally, the results are commented in terms of splat morphology and heat flux from the droplet towards the substrate.

## 2. Multi impact modeling

### 2.1. Physical modeling

This paper deals with the impact, spreading and solidification of several droplets onto the solid substrate. The domain is a box, containing the substrate, the plasma gas and the droplets. This 3D domain is small enough to focus on the impact of three particles, impacting at random positions, at a known frequency. The physical properties of the materials are presented in Table 1. As a first approach, the properties are considered constant: indeed, the aim of the article is to describe the thermal and dynamic behaviors of impacting droplet, and the induced cooling rate in the present configuration leads to a low variation of physical properties, which will be considered in future studies. Moreover, the liquid–solid phase change method is based on the Stefan–Neumann model which considers a constant density. The surface tension is set at $\sigma = 0.5\ \mathrm{N\ m^{-1}}$.

The motion of the droplet and of the surrounding gas is modeled by Navier–Stokes equations, assuming a compressible gas flow and an incompressible droplet. The mass conservation is usually expressed under the form of Eq. (1).

$$\frac{\partial \rho}{\partial t} + \nabla(\rho.\mathbf{u}) = 0 \tag{1}$$

The compressibility is a challenging numerical problem. This equation has been modified to correctly solve the flow: the gas is assumed to be perfect. The isothermal compressibility $\chi^T$ is introduced to perform a direct link between the pressure and the velocity (Eq. (2)). This equation and the numerical treatment have been developed by Caltagirone et al. [13].

$$\frac{\partial p}{\partial t} = -\frac{1}{\chi_T}\nabla(\mathbf{u}) - \mathbf{u}.\nabla(p) \tag{2}$$

The surface tension effect is introduced in Eq. (3) thanks to the local droplet–gas interface curvature, following the continuum surface force (CSF) model introduced by Brackbill et al. [14].

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}.\nabla\mathbf{u}\right) = \rho\mathbf{g} - \nabla p + \nabla\left(\mu\left(\nabla\mathbf{u} + \nabla\mathbf{u}^T\right)\right) + \sigma\mathbf{n}\kappa\delta + \frac{\mu}{K}\mathbf{u} \tag{3}$$

The last term of Eq. (3) is linked to the local permeability $K$, which is used to model the substrate: the permeability $K$ takes a very low value (typically $10^{-20}\ \mathrm{m^2}$) in the substrate so that the velocity is penalized to zero. The momentum equations (Eq. (3)) are directly linked to the definition of the droplet/gas interface, since the term $\sigma\mathbf{n}\kappa\delta$ is not null only at the interfacial position. The parameters $\mathbf{n}$, $\kappa$ and $\delta$ represent respectively the normal to the interface, the local curvature and the Dirac function used to localize the droplet gas interface. The interface geometry is built over time by an advection equation of the phase function: for each representative element volume (REV), the volume fraction of the droplet is given by:

$$\Phi = \frac{V_{droplet}}{V_{ER}} \tag{4}$$

In expression (4), $V_{droplet}$ is the volume of droplet material in the REV, and $V_{ER}$ is the volume of the total REV. Thus, if the droplet fills the REV entirely, $\Phi = 1$, whereas $\Phi = 0$ corresponds only to the gas. The REV where $0 < \Phi < 1$, contains the droplet/gas interface. The time and space evolution of $\Phi$ is given by an advection equation (Eq. (5)):

$$\frac{\partial \Phi}{\partial t} + \mathbf{u}.\nabla\Phi = 0 \tag{5}$$

A static contact angle $\theta = 120°$ is imposed, following the $\Phi$ smoothing technique developed by Guillaument et al. [16]. Concerning heat transfer, convection is the main transfer mode in the droplet. Energy is conveyed to the substrate by conduction. The energy equation is solved to model all heat transfer (except radiation assumed as negligible due to the low temperature), including the phase change (Eq. (6)).

$$\rho c_p\left(\frac{\partial T}{\partial t} + \mathbf{u}.\nabla T\right) = \nabla(\lambda\nabla T) + S_C \tag{6}$$

The term $S_C$ in Eq. (6) is related to the phase change that occurs at a given melting temperature $T_m$. The solid fraction $f_s$ is locally defined as:

$$\begin{cases} f_s = 0 & \text{if } T > T_m \\ 0 < f_s < 1 & \text{if } T = T_m \\ f_s = 1 & \text{if } T < T_m \end{cases} \tag{7}$$

The relation between the source term $S_C$ and the solid fraction $f_s$ is given by Eq. (8) through the latent heat $L_f$.

$$S_C = \rho L_f \frac{\partial f_s}{\partial t} \tag{8}$$

A thermal contact resistance (RTC) is included to represent the non perfect contact between the droplets and the substrate. The local thermal conductivity is modified between the two materials to limit the heat transfer, with a constant value: $RTC = 5 \cdot 10^{-6}\ \mathrm{m^2\,K\,W^{-1}}$. Vardelle et al. [17] have shown that this parameter and the splat thickness are linked. They found that the RTC could vary between $10^{-8}$ to $10^{-6}\ \mathrm{m^2\,K\,W^{-1}}$. The present study proposes a large value, and future studies will be based on the analysis of this specific parameter.

$$\lambda = \frac{\Delta z_1 + \Delta z_2}{\frac{\Delta z_1}{\lambda_1} + \frac{\Delta z_2}{\lambda_2} + \frac{RTC}{\Delta x \Delta y}} \tag{9}$$

In Eq. (9), $\Delta x$, $\Delta y$ and $\Delta z$ are respectively the mesh size in horizontal directions $x$ and $y$ and the vertical direction $z$. Indices 1 and 2 refer respectively to the substrate and the droplet materials.

**Table 1**
Physical properties of materials.

| | Density [kg m$^{-3}$] | Specific heat [J kg$^{-1}$ K$^{-1}$] | Conductivity [W m$^{-1}$ K$^{-1}$] | Viscosity [Pa s] | Latent heat [J kg$^{-1}$] | Melting temperature [K] |
|---|---|---|---|---|---|---|
| Substrate | 7900 | 477 | 14.9 | – | – | – |
| Droplet | 5700 | 604 | 2.32 | 0.03 | 706860 | 2950 |