Deformation behavior of a liquid droplet impacting a solid surface

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Abstract: The quality of coatings obtained by means of thermal spraying depends strongly on the mechanism of the interaction between the molten droplets and the surface to be covered. The aim of the present study is to simulate the impact of a droplet onto a substrate, in order to have a good understanding of the dynamics of droplets impact. In this study, the process of droplet spreading is described; the effect of impact velocity on the dynamic of impact is studied with a wide range of wettability. The pressure, velocity and spreading factor during the droplet spreading are reported.
Finite elements analysis using the COMSOL multiphysics is used in this simulation. The results obtained are in excellent agreement with previously published results, experimentally and theoretically.

Keywords: droplet impact, multiphase flow, free surface, level set;

1. Introduction

Thermal spray technology is the term which means the family of all processes of surface treatment that consisting of the production of functional coatings (20 µm to several mm) on technical surfaces using different heat sources. Theses coatings are used against all forms of wear, such as abrasion, erosion and corrosion and also to provide a thermal protection [1,2]. These techniques have been developed and optimized for more than 30 years, especially the plasma spraying technique which is the most versatile of the thermal spray processes thanks to its capability of spraying all different kinds of materials such as metals, ceramics, cermets, etc. This technology has been remarkably successful in even the most demanding applications such as aeronautic, aerospace, nuclear, etc.
In plasma spraying, the coatings are obtained by injecting particles of material into a plasma jet, where they are melted and projected at high speed toward a prepared surface on which they flatten, quench rapidly and solidify. Coating is built up when millions of individual molten droplets are cumulatively deposited on the top of each other layer by layer, which leads to a multilayer structure[3,4,5,6,7]. Many properties of the sprayed coatings, especially the adhesive strength to the substrate depend greatly on the splat behavior of the dynamics of flattening the molten powder particles. So a better understanding of the dynamics of the collision between the droplets and the substrate is required, to understand the microstructure of these coatings and thus to control their quality.
The impact and spreading of a liquid droplet on a solid surface has been extensively evaluated, using the spreading factor, ξ=D/d, that is, the ratio of the diameter of spherical particle before the impact, d, to that of final disk splat, D. The evolution of the flattening degree is usually used to describe the droplet evolution
In this study, A numerical multiphase flow model using finite elements analysis has been proposed to simulate the impact and the spreading of a droplet onto a substrate, taking into account the effect of the impact velocity and the wettability which are particularly the important parameters necessary to understand, clarify thus to control the flattening mechanism. The pressure, velocity and the spreading factor during the droplet spreading are reported. This model is implemented in the COMSOL software package.

2. Model and simulation

The process of the impact and deformation of droplets onto a solid surface is a very complex process that encompasses fluid dynamic, physics, and free surface. Figure 1 shows the geometry of the problem and the initial configuration at t = 0 ms: a spherical water droplet of a diameter D_0 =3 mm, which impacts at a velocity V_0 =1,18 m/s onto a solid surface at a normal incidence. The equilibrium contact angle chosen is 120°.

The droplet has a density of 997 kg/m^3 and a viscosity of 1.10^{-3}Pa.s. For the surrounding gas (air) the density and the viscosity have values of 1,3 kg/m^3 and 1,7 10^{-5}Pa.s respectively. The liquid-gas surface tension have a value of σ = 0,073 N/m. For reasons of symmetry only the droplet half is modeled and the flow is modeled using 2D axis symmetric model. The coordinate system is represented by the radial and axial coordinates (r,z) and we assumed that both fluids are incompressible and Newtonian. It is assumed that the surrounding gas has no effect on the deposition process.

In this simulation, full Navier-Stokes equations have to be considered (Eq1 and Eq2):

$$\rho\frac{\partial u}{\partial t}+\rho(u\nabla)u=-\nabla p+\nabla.\mu(\nabla u+(\nabla u)^T)+\rho g+F_{TS} \qquad \textbf{Eq. 1}$$

$$\nabla u = 0 \qquad \textbf{Eq. 2}$$

u is the velocity, p, ρ and μ are respectively the pressure field, density and kinematic viscosity of each fluid, g is the gravitational acceleration and F_{TS} represents the capillary forces given by:

$$F_{TS} = \sigma.k.\delta.n \qquad \textbf{Eq. 3}$$

where σ, δ and k are respectively the surface tension coefficient, the Dirac function and the average local slop of the curve at the liquid-gas interface. n is the normal at the liquid-gas interface. Other assumptions are that the liquid is incompressible and the fluid flow is laminar.

To track and follow the evolution of the interface between the two fluids (liquid and air), we have used the level set method [8] which has proven popular in recent years for tracking, modeling and simulating the motion of moving interfaces or boundaries. In this method, the interface is represented by a certain level set or iso-contour of a globally defined function: the level set function ϕ. This function ϕ is a smoothed step function that equals (0) in a domain and (1) in its complementary part. Across the interface, there is a smooth transition from (0) to (1) and the interface is represented implicitly by the 0,5 iso-contour (Fig.1). The interface moves with the fluid velocity u. This is described by the following equation:

$$\frac{\partial \phi}{\partial t}+\mathrm{u}.\nabla\phi=\gamma\nabla.(\varepsilon\nabla\phi-\phi(1-\phi)\frac{\nabla\phi}{|\nabla\phi|}) \qquad \textbf{Eq. 4}$$

The terms on the left-hand side of equation 4 give the correct motion of the interface, while those on the right-hand side are necessary for numerical stability. The parameters ε and γ determine the thickness of the region and the amount of re-initialization or stabilization of the level set function respectively. Any property α of the two fluids at the interface such as density, viscosity or thermal conductivity may be expressed as:

$$\alpha = \alpha_{gaz} + \phi(\alpha_{liquide} - \alpha_{gaz}) \qquad \textbf{Eq. 5}$$

This model is solved by the finite elements method and by using Comsol multiphysics 3.5a software [9] which is a powerful tool for the simulation of engineering problems based on Partial Differential Equations (PDEs).

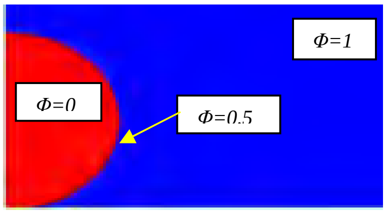

Figure 1. Initial configuration of the droplet at t=0 ms (time of impact) and the surface and contour plot of the initialized level set function

3. Results and discussion

3.1. Validation of the model and droplet impact observations

Figure 2 shows the different stages of a 3 mm water droplet impacting a solid surface with a velocity of V_0=1.18 m/s, in 2D (Fig2a) and 3D simulations (Fig 2b). The results agree well with those carried out experimentally by R.Rioboo [10] (Fig 2c).

The droplet has a spherical shape before impact, and immediately after impingement, it starts to spread. A lamella (a thin film) forms at the solid surface, develops and expands horizontally with a radial velocity higher than that before impact. Thus its diameter increases very rapidly while its thickness decreases as shown in Figure 3.

Indeed when the droplet enters in collision with the solid surface, it undergoes a very high compression and a shock wave generates and proceeds upward inside the droplet (Fig.4), because the droplet is assumed as an incompressible fluid, so the fluid between the centre of the droplet and the solid substrate is compressed at the moment of impact.

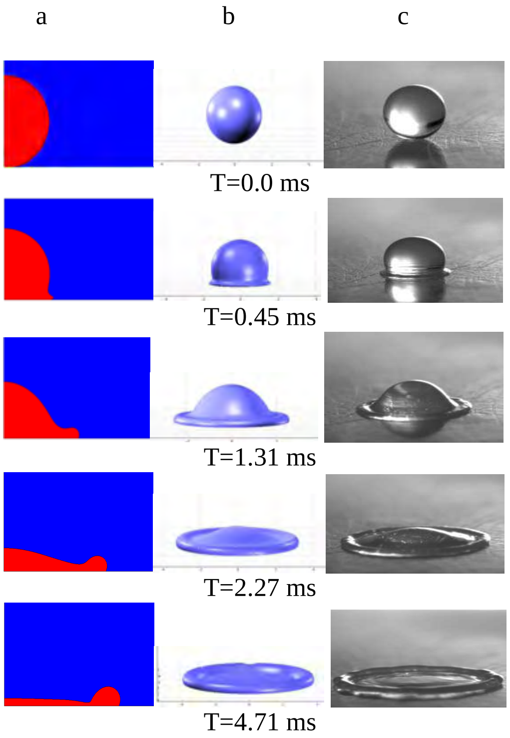

Figure2. Impact and flattening of a 3 mm water droplet with a velocity V0= 1.18 m/s, (a) 2D simulation, (b) 3D simulation and (c) experimental results carried out by R.Rioboo [10].

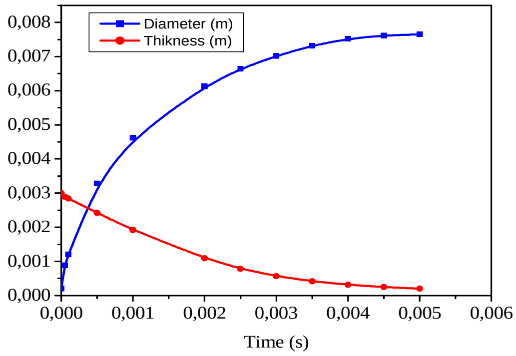

Figure 3. Evolution of droplet diameter and thickness versus time

This compression is observed upon the impact just on the liquid zone adjacent to the solid surface, while the rest of the droplet is still far for this compression (Fig.4). The elastic energy on the compressed liquid gradually transferred into kinetic energy of lateral flow. The lateral jetting velocity increased to a value two to five times greater than the impact velocity [11], in this simulation the lateral flow velocity at the first instants of impact is about three times that one before impact.

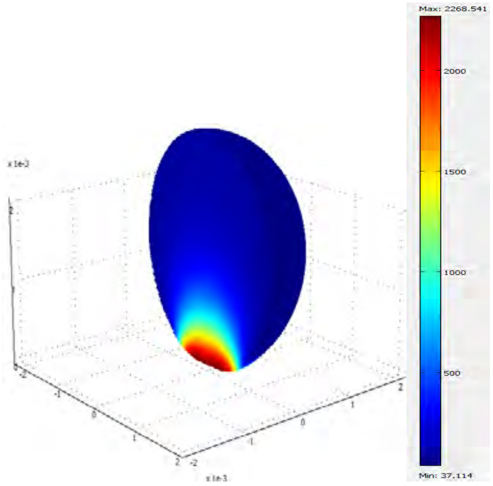

Figure4. The pressure distribution into the droplet at the moment of the impact

The droplet reaches its maximum spread at 4.7 ms, a raised rim is formed at the periphery of the lamella due to the accumulation of the mass by the surface tension forces which limit the spread and decelerate the motion of the splat at the periphery. Figure 5 shows that the velocity at the edge of the droplet at the end of spreading, exactly at t=4.8 ms, has a component in the negative r axis, which makes the droplet begin to recoil under surface tension forces.

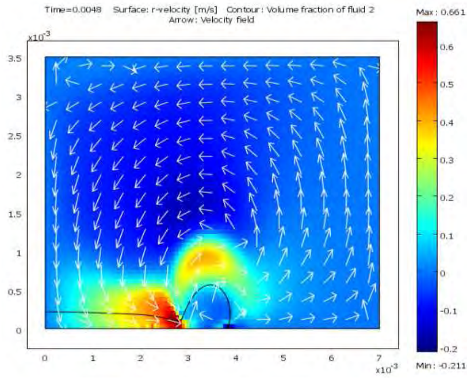

Figure5. Velocity field at t=4.8 ms (time of recoiling start)

The spreading factor ξ_{max}, given by normalizing the splat diameter D to the initial droplet diameter D_0 plays an important role for the validation of the simulation codes of droplets impact. The value of ξ_{max} determined in the present work is $\xi_{max}= D/D_0 = 2{,}53$. Pasandideh-Fard et al [12] have developed an analytical model (Eq 6) to predict the maximum spread factor at the end of the droplet impact using the mass and energy conservation before and after the impact. They estimated that their results may be compared with those in the literature with an error less than 15%. Our results concerning the spreading factor values compare well with those determined using Pasandideh-Fard analytical model (Eq. 6) within a deviation less than 7%.

$$\xi_{\max} = \sqrt{(We+12)/3(1-\cos(\theta))+4(We/\sqrt{\mathrm{Re}})} \qquad \textbf{Eq. 7}$$

$$\mathrm{Re} = \rho.d.u/\mu \ \text{ et } \ We = \rho.d.u^2/\sigma$$

Where We is the Weber number ($We=\rho.d.u^2/\sigma$), Re is the Reynolds number ($Re= \rho.d.u/\mu$) and θ is the contact angle.

3.2. Effect of impact velocity and wettability

To be close to the parameters used in thermal spraying, we use a micrometric droplet (D= 10 µm) to investigate the effect of the impact velocity and the wettability.
Figure 6 shows the droplet at the end of the flattening of a micrometric droplet (D= 10 µm) for different values of impact velocity and wattability.

It was observed that impact velocity has a significant effect on droplet spreading; it produces significant changes in the shape of the splat. Whatever the value of the wettability, increasing the impact velocity leads to increase the spreading time and also the diameter of the droplet thus spreading factor ξ_{max}.
Figure7 shows the effect of impact velocity on the spreading factor for a fixed value of the contact angle (θ = 45°), once the spreading factor ξ_{max} reaches a maximum value, it begins to decrease since the droplet retracts and recoils owing to the surface tension forces. For high impact velocities, the phenomenon of splashing occurs; droplets are ejected from the rim of the lamella at the end of flattening, because of the important kinetic energy which exceeds the surface tension forces. The number of these droplets increases with increasing the impact velocity

Despite of several authors who have neglected its effects, the wettability remains a key factor in the process of droplet impacts. In this study we have tacked into consideration the effect of this phenomenon by introducing the equilibrium contact angle θ.

Figure 6 shows the effect of the impact velocity on the shape of the splat at the end of flattening for surfaces of different wettabilities. From this figure, it's obvious that the wettability has an effect on the shape of the splat, notably on the thickness and the maximum diameter and thus on the spreading factor and spreading time.

Whatever the value of the impact velocity, increasing the contact angle leads to increasing the splat thickness at the end of flattening and to decreasing the spreading factor (Fig6Figure). The effect is more important when increasing the impact velocity.

It was also seen that, for a lower impact velocity (for example v=10 m/s), the recoil of the droplet occurs readily and rapidly for the surfaces with high contact angle and the time of spreading is very short but for high impact velocities the droplet spreads without recoil.
The main remark in this simulation is that the splashing depends on the wettability; it occurs

early when the system is less wetted. For example the splashing occurs at the impact velocity of 50 m/s when the contact angle is 120°, while it occurs at 60 m/s when the contact angle is 10°.

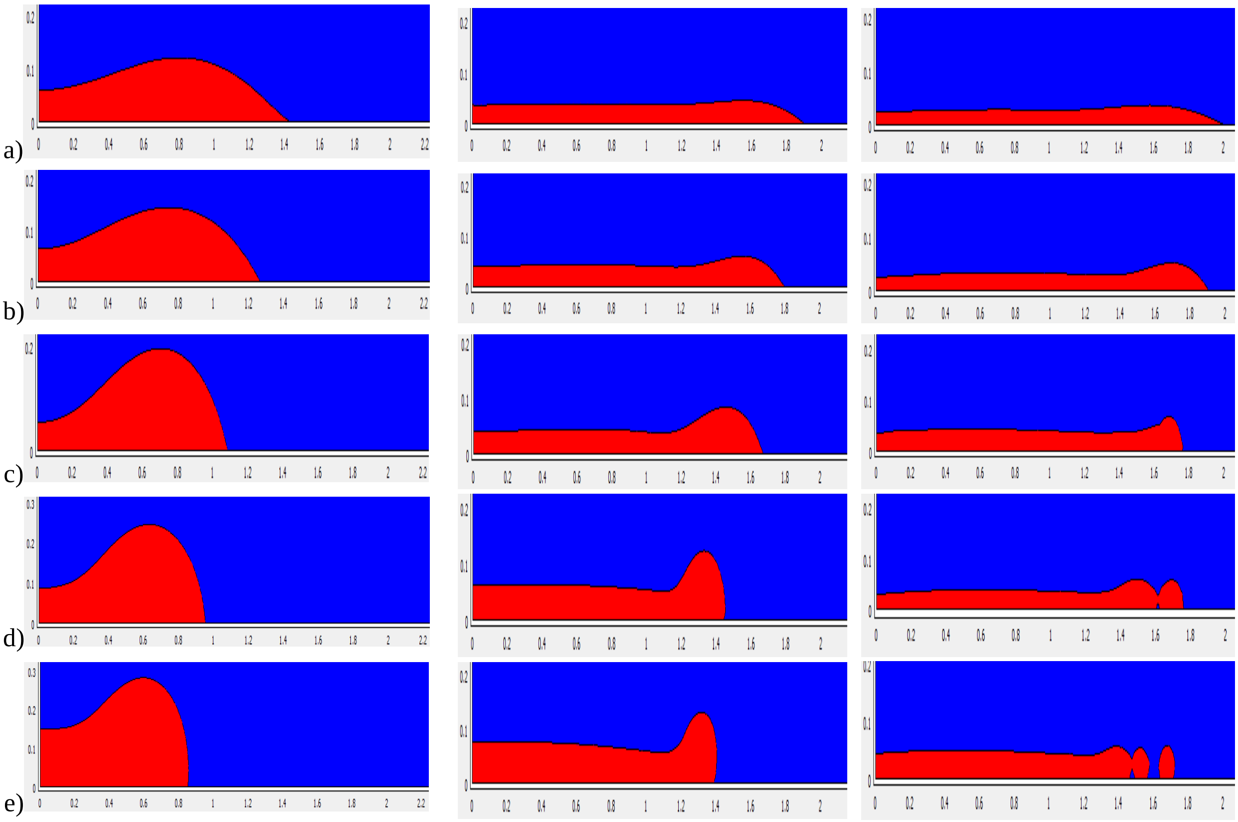

Figure6. Morphologies for the splat at the end of the flattening for different values of the impact velocity and the contact angle: a)θ=10°, b)θ=40°, c)θ=60°, d)θ=80°, e)θ=100°

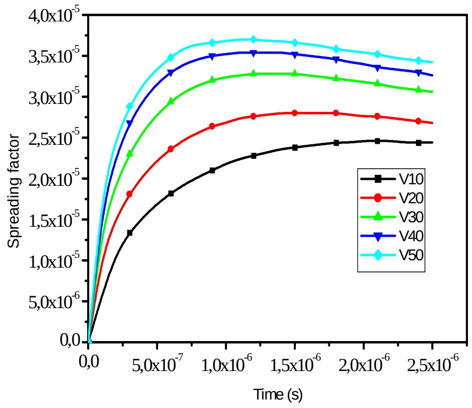

Figure7. Spread factor evolution during the flattening for different impact velocities.

The impact pressure is strongly influenced by the impact velocity as shown in figure8, which shows the pressure at the impact for different impact velocities at the point (r=0,z=0). For example for a velocity of 20 m/s the pressure at the impact is 6,83 10^5 Pa and reaches 2,09 10^7Pa when the velocity is increased to 120 m/s.

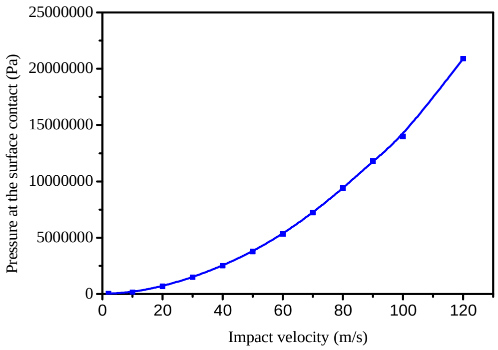

Figure8. Pressure at the contact point (r=0, z=0) for different impact velocities.

4. Conclusion

The impact of a droplet onto a rigid substrate was simulated using Comsol multiphysics 3.5a. The results agree well with those obtained analytically and experimentally.

It was shown that the impact velocity and wettability have a significant effect on the dynamics of droplet impact especially on the spreading factor and also on time of droplet spreading.

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