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Massively parallel multiphase simulation of the impingement and solidification of multiple submicrometer droplets in suspension plasma spraying process

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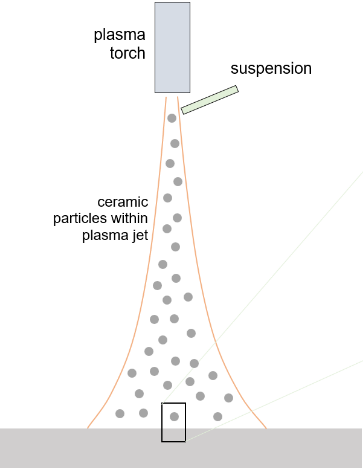
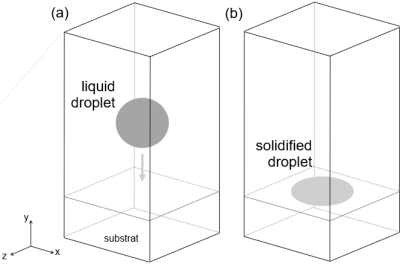
Droplet impact and solidification in suspension plasma spraying





plasma temperature > 3000 K
substrate temperature = 523 K (if preheated)

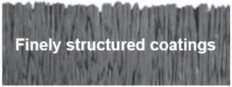


image extract: Clarke et al. (2012)

Multiphase compressible model with liquid-solid phase change

Compressible ideal gas and incompressible liquid

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

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) + C \frac{f_s^2}{(1 - f_s)^3 + b} \mathbf{u} = -\nabla p + \nabla \cdot \boldsymbol{\tau} + \sigma \kappa \nabla f_d \tag{2}$$

$$\frac{dp}{dt} = -\rho c^2 \nabla \cdot \mathbf{u} + \frac{\beta_p \rho c^2}{\rho c_p^*} \left(\nabla \cdot (\lambda \nabla T) + \rho L \frac{\partial f_s}{\partial t} \right) \tag{3}$$

$$\frac{\partial H}{\partial t} + \nabla \cdot (\mathbf{u} H_f) = \frac{dp}{dt} + \nabla \cdot (\lambda \nabla T) \tag{4}$$

$$\frac{\partial f_\ell}{\partial t} + \mathbf{u} \cdot \nabla f_\ell = 0 \tag{5}$$

where subscripts d = droplet, ℓ = liquid, s = solid, f = fluids

→ Carman-Kozeny for solid PCM ; CSF model for surface tension ; MOF or conservative VOF

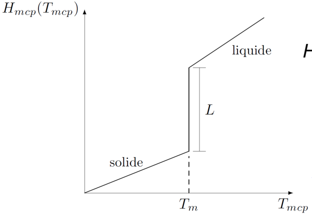
→ ⓐ **linearized enthalpy method for the liquid-solid phase change**

→ ⓑ **incremental pressure correction method for compressible flows** ($\phi = p^{n+1} - p^n$)

→ no contact angle imposed (high We, immediate solidification at contact), no turbulence considered

ⓐ Linearized enthalpy method

Pure PCM: isothermal liquid-solid phase change model in terms of volumetric enthalpy ($H = \rho h$)



$$H_{pcm}(T_{pcm}) = \begin{cases} \rho_s c_{p,s} T_{pcm} & T_{pcm} < T_m \\ \rho_s c_{p,s} T_{pcm} + \rho_s(1 - f_s)L & T_{pcm} = T_m \\ \rho_s c_{p,s} T_{pcm} + \rho_s L + \rho_\ell c_{p,\ell}(T_{pcm} - T_m) & T_{pcm} > T_m \end{cases} \quad (6)$$

$$\left.\frac{dH}{dT}\right|_{pcm} = \left.\rho c_p^*\right|_{pcm} \quad (7)$$

→ derivative undefined at T_m, we use $dH/dT|_{pcm}$ = 0.5($\rho_s c_{p,s} + \rho_\ell c_{p,\ell}$)*coeff

note : dH/dT equal to ρc_p for incompressible & ideal gas

The idea: linearization of the enthalpy-temperature relation by first order Taylor expansion around a previously known value of the temperature (sub-iteration $k - 1$) – from Kaaks et al., 2022 & other authors

$$H_k^{n+1} = H_{k-1}^{n+1} + \left.\frac{dH}{dT}\right|_{k-1}^{n+1} [T_k^{n+1} - T_{k-1}^{n+1}] \quad (8)$$

→ **used to develop the energy equation (4) from enthalpy to temperature form, e.g:**

$$\left.\rho c_p^*\right|_{k-1}^{n+1} \left(\frac{T_k^{n+1} - T_{k-1}^{n+1}}{\Delta t} + \mathbf{u} \cdot \nabla T^n \right) = T_k^{n+1} \beta_p \frac{dp^{n+1}}{dt} + \nabla \cdot (\lambda \nabla T_k^{n+1}) + \frac{H^n - H_{k-1}^{n+1}}{\Delta t} \quad (9)$$

Pressure equation

Considering pressure $p = p(\rho, T)$

$$dp = \left.\frac{\partial p}{\partial \rho}\right|_T d\rho + \left.\frac{\partial p}{\partial T}\right|_\rho dT \tag{10}$$

using continuity equation, isothermal compressibility and thermal expansion coefficients

$$\frac{dp}{dt} = -\frac{1}{\chi_T}\nabla \cdot \mathbf{u} + \frac{\beta_p}{\chi_T}\frac{dT}{dt} \tag{11}$$

and in conjuction with the energy equation as well the thermodynamic relations

$$\gamma = \frac{(\partial h/\partial T)_p}{(\partial e/\partial T)_v}\ ,\ \chi_T = \frac{\gamma}{\rho c^2} \text{and } \frac{T\beta_p^2}{\rho c_v \chi_T} = \gamma - 1 \tag{12}$$

we have the equation

$$\frac{dp}{dt} = -\rho c^2 \nabla \cdot \mathbf{u} + \frac{\beta_p \rho c^2}{\rho c_p^*}\left(\nabla \cdot (\lambda \nabla T) + \rho L \frac{\partial f_s}{\partial t}\right) \tag{13}$$

ⓑ Incremental pressure correction method

Obtaining a predicted velocity $\mathbf{u}^*$ from pressure gradient at time n, e.g.

$$\rho^n \frac{\mathbf{u}^* - \mathbf{u}^n}{\Delta t} = -\nabla p^n + F^* \tag{14}$$

Goda's classical approach : difference between equation (14) and momentum equation (2) and neglecting nonlinear and stress tensor divergence

$$\mathbf{u}^{n+1} - \mathbf{u}^* = -k_\phi \nabla \phi \tag{15}$$

$$\phi = p^{n+1} - p^n \tag{16}$$

then applying divergence

$$\nabla \cdot \mathbf{u}^{n+1} - \nabla \cdot \mathbf{u}^* = -\nabla \cdot (k_\phi \nabla \phi) \tag{17}$$

Combining pressure equation (13) and equation (16), we have the **pressure correction equation**

$$\frac{\phi}{\rho c^2 \Delta t} - \nabla \cdot (k_\phi \nabla \phi) = -\nabla \cdot \mathbf{u}^* + S \tag{18}$$

When $c \to \infty$ and $\beta_p = 0$, equation (17) is reduced to incompressible flow

Step-by-step

1. velocity prediction

$$\rho^n \frac{\mathbf{u}^* - \mathbf{u}^n}{\Delta t} = -\nabla p^n + F^*$$

2. pressure increment field resolution

$$\frac{\phi}{\rho c^2 \Delta t} - \nabla \cdot (k_\phi \nabla \phi) = -\nabla \cdot \mathbf{u}^* + S$$

3. velocity and pressure update

$$\mathbf{u}^{n+1} = \mathbf{u}^* - k_\phi \nabla \phi$$

$$p^{n+1} = p^n + \phi$$

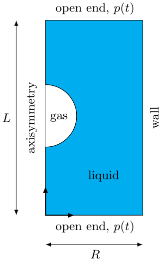
4. solve temperature

$$\rho c_p^* \Big|_{k-1}^{n+1} \left(\frac{T_k^{n+1} - T_{k-1}^{n+1}}{\Delta t} + \mathbf{u} \cdot \nabla T^n \right) = T_k^{n+1} \beta_p \frac{dp^{n+1}}{dt} + \nabla \cdot (\lambda \nabla T_k^{n+1}) + \frac{H^n - H_{k-1}^{n+1}}{\Delta t}$$

5. solve advection (conservative VOF-PLIC method)
6. update physical parameters through EoS(T^{n+1}, p^{n+1})

Computational Fluid Dynamics

Bubble expansion under variable pressure



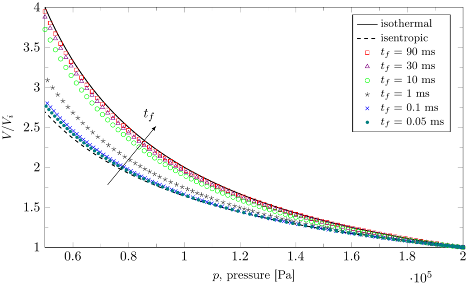
L = 4 mm, R = 2 mm

- compressible ideal gas
- incompressible liquid
- p_o = 0,2 MPa, p_f = 0,05 MPa
- pressure variation

$$p(t) = p_o - \frac{p_o - p_f}{t_f} \times t$$

- t_f = 0,05, 0,1, 1, 10, 30, 90 ms
- T_o = 300 K
- 256 × 512 mesh
- MOF method
- O2 centered (momentum, energy)
- O2 uncentered (pressure)

→ simulations should give real expansion between ideal isothermal and isentropic curves

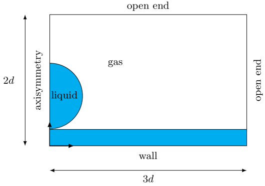


→ larger t_f tending towards isothermal

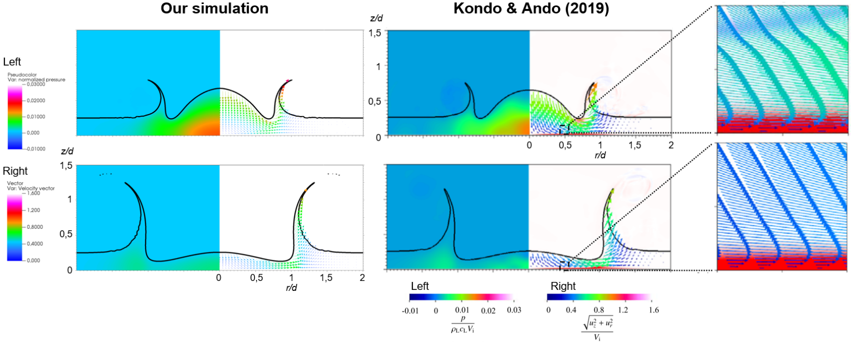
→ lower t_f tending towards isentropic

reference : Urbano (2022)

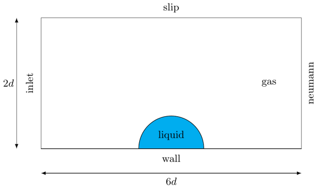
Micrometer droplet impact to liquid film



- compressible ideal gas
- weakly compressible liquid considered as stiffened gas
- d = 200 µm, v_d = 50 m/s, p_o = 101325 Pa
- mesh 1200 $\times$ 800 ; MOF method
- O2 centered (momentum) and TVD (pressure) schemes



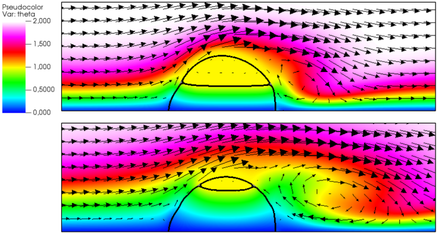
Drop solidification with forced convection



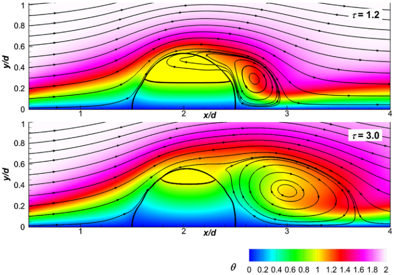
- incompressible case with liquid to solid phase change
- compressible method, Re = 400, Pr = 0.01, St = 0.1, Ca = 0.01
- mesh 300 $\times$ 100 ; conservative VOF method
- WENO3 (momentum, energy) and TVD (pressure) schemes

note: ρ_s / ρ_ℓ = 1.0 (our case), ρ_s / ρ_ℓ = 0.9 (reference)

Our simulation

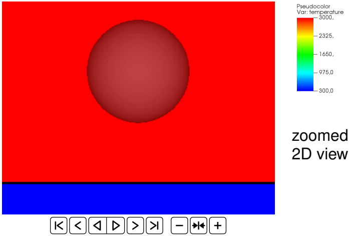


Vu (2018)

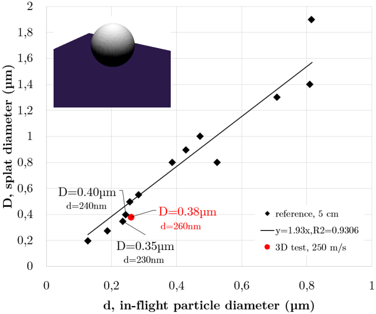


3D simulation

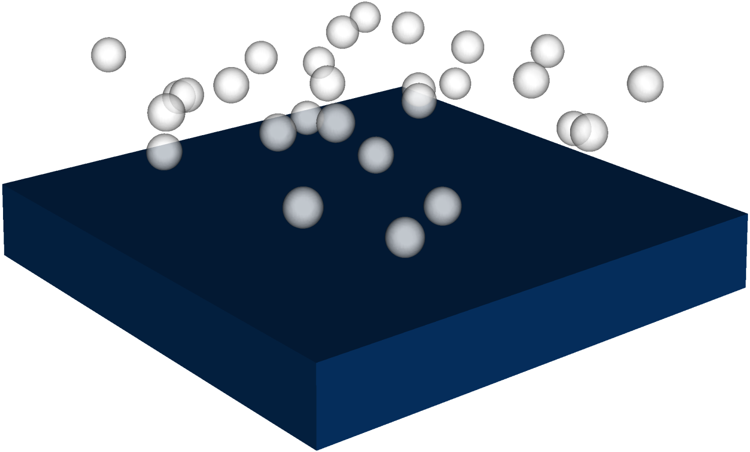
- 0.26 µm zirconia droplet, Re = 10.9, We = 185.25
- considered real experimental conditions by Fazilleau (2003)
  - – optimal distance from torch around 5 cm, thus having same initial velocities within the droplet and the plasma gas
  - – velocity of 250 m/s observed for 100 nm to 5 µm droplets
  - – same properties considered for zirconia, T_m = 3000 K
  - – plasma gas Ar-H2 also considered as ideal gas
  - – glass substrate not preheated (300K), non-perfect contact (e.g. RTC = 1e-6) so that no substrate melting
  - – T_o = 3800 K for fluids (average of plasma and droplets)
- partial rarefaction: mean free path of $\leq$ 2.47 µm for plasma gas at $\leq$ 3800 K and thus Kn $<$ 10 within transition regime
  - – to apply continuum model : Maxwell slip on substrate combined with an effective viscosity model by Beskok & Karniadakis (1999)
- quarter domain 0.75$\times$1.2$\times$0.75 µm^3, 60$\times$96$\times$60 mesh
- conservative VOF, WENO3 (momentum, energy) and TVD (pressure) schemes
- the Neumann boundary conditions around the domain can cause non-physical recirculations of the gas phase



zoomed 2D view



Simulation of 52 YSZ droplets



d = 1 µm
v = 100 m/s

Re = 26.34
We = 116.17

15×15 µm^2
SS surface

34.56M points,
512 processors
at the MCIA

Conclusion

1. Necessity of better initialization of velocity, pressure and temperature
2. Necessity of improvements at the boundary conditions to avoid non-physical pressure reflection
3. Great potential of current methods for multiple droplet impact simulation in suspension plasma spraying
4. Possible simulation of hundreds to thousand of submicrometer droplets at a surface of 30×30 μm^2 with 2048 processors
5. Entry data of actual diameters and velocities (as well as spatial and temporal distribution of droplets) at real operating conditions can allow better and larger simulations - tens of thousands droplets - with increasing capacity of supercomputers and GPU solvers
6. Research may be extended to the use of stochastic methods coupled with an IA to reconstruct interface splats of droplets (trained with 3D simulations)

Thank you