# Numerical simulation of flake orientation during droplet impact on substrates in spray painting processes

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Metallic pigment





Optical impression of a metallic effect paint

Aim of the Research :

- How do flakes/pigments orientate themselves and how can this be controlled
- Investigation of flake orientation by droplet impact processes





# Information about droplet size and impact velocity in spray painting processes

atomizer	D <sub>32</sub> (µm)	Impact velocity U (m/s)
Airless	68	10
pneumatic	8	2
Rotary bell	17	1.5



Typical paint droplet size distribution



Ref. Q. Ye, J. Domnick, Analysis of droplet impingement of different atomizers used in spray coating processes, J. Coat. Technol. Res., 14 (2) 467–476, 2017

- Fine droplets with pneumatic gun
- For droplet D < 50µm, impact velocity U < 10 m/s</p>
- Important parameter for the current study should be:

 $U < 10 \text{ m/s}, D = 50 \mu \text{m}$  ( if so, 20 $\mu \text{m}$ , 100 $\mu \text{m}$  and 300 $\mu \text{m}$ )





- 3D time-dependent VOF simulation (Ansys\_Fluent CFD code was applied)
- Dynamic contact angle model validated by measurement

$$\theta_{D} = \begin{cases} v_{cl} > 0 & \theta_{A}(120^{\circ}) \\ \overline{v_{cl}} < |\delta| \cap v_{cl} < \delta & \theta_{int} = 90^{\circ} \\ \theta_{\nabla\phi} < \theta_{A} & \theta_{\nabla\phi} \\ \theta_{\nabla\phi} \le \theta_{E} & \theta_{E} \end{cases} \quad \text{where } \delta = -0.1$$

Rigid body motion equations for calculating flake movement (user-defined functions)

$$\vec{F}_p = \int_A p(\vec{r}) \, \vec{n} dA \cong \sum_{r_f}^{n_f} p_c \vec{A}_f \quad \text{wobei} \quad \vec{A}_f = \vec{n}_f A_f$$
$$\vec{F}_\tau = \int_A^A \vec{\tau} dA \cong \sum_{r_f}^{n_f} \vec{\tau}_f A_f$$
$$\vec{M} \cong \sum_{r_f}^{n_f} (\vec{r}_f - \vec{r}_s) \times \left(\vec{F}_p + \vec{F}_\tau\right)_f$$

Calculating forces and moments

$$\Delta \vec{v} = \int_{t}^{t+\Delta t} \dot{\vec{v}} dt = \int_{t}^{t+\Delta t} m^{-1} \left( \vec{F_p} + \vec{F_\tau} + m\vec{g} \right) dt$$
$$\Delta \vec{\omega} = \int_{t}^{t+\Delta t} \dot{\vec{\omega}} dt = \int_{t}^{t+\Delta t} \mathbf{I}^{-1} \left( \vec{M} - \vec{\omega} \times \mathbf{I} \cdot \vec{\omega} \right) dt$$

Time integration using Adams-Moulton algorithm of 4th order

I ~1.6×10<sup>-23</sup> [kg·m<sup>2</sup>] that is too small for 6DOF motion solver by ANSYS





Dynamic mesh with overset-method, 3-dimentional model with symmetry boundaries, the maximum computational domain: 8D × 8D × 3D





Domain mesh overlaid with component mesh



Contours of VOF overlaid with mesh at t = 0 s, blue: liquid, red: air





μm³

Component mesh with flake 1x16x16

### Basic simulation methods

- D/ $\Delta x = 150$  obtained after the study of grid independence
- Dynamic mesh adaption
- Typical time steps of 0.01 0.1 μs
- Parameters

Droplet diameter D (µm)	<mark>50</mark> , 100, 300
Droplet velocity U (m/s)	0.5 - 10
Liquid viscosity η (Pas)	0.01 – 0.04 and shear thinning viscosity
Surface tension $\sigma$ (N/m)	<mark>0.025</mark> , 0.063
Liquid density ρ (kg/m <sup>3</sup> )	1020,1200
Static contact angle (°)	50 - 60



#### Mesh distribution using dynamic mesh adaption

Height of film (µm)	30, <mark>60</mark> , 100
Flake size (µm <sup>3</sup> )	1×16×16
Flake density (kg/m <sup>3</sup> )	3200
Re-number, Re= $\rho$ UD/ $\eta$	5 – 100
We-number, We = $\rho U^2 D/\sigma$	3 – 1200
Oh-number, Oh = $\eta / \sqrt{(\sigma D \rho)}$	0.1 – 2.2





Droplet impact on dry surfaces using dynamic contact angle model











Evolution of the droplet contour and flake orientation ( D= 100  $\mu$ m,  $\eta$  = 20 mPas, U = 6m/s,  $\sigma$  = 0.063 N/m )



Comparison of flake orientation with different viscous droplets.



Newtonian droplet: D=50 $\mu$ m,  $\sigma$  = 0.025 N/m,  $\eta$  = 20 mPas, h\_film = 60 $\mu$ m

Impact velocity U = 0.5 m/s



Impact velocity U = 10 m/s



Droplet deposition, final angle =  $32^{\circ}$ 

Cratering, final angle = 49.3°

Outcome of droplet impact on wet surface by spray paintng:

- Deposition
- Cratering
- Crater/crown





Comparison of flake orientations by droplet impact on the wet solid surface using different viscous droplets ( $H_f = 60 \mu m$ ,  $D = 50 \mu m$ ) Initial position  $\Im$ 



At quasi-static state:

- Viscosity  $\uparrow \rightarrow$  Angle  $\uparrow$
- For lower viscosity, U  $\uparrow \rightarrow$  Angle  $\uparrow$

- Effect of surface tension is weak for the final angle
- Effect of film thickness (H/D > 0.5) is weak





Simulation with shear thinning viscosity (D = 50  $\mu$ m, U = 5m/s,  $\sigma$  = 0.025 N/m, h\_film = 60 $\mu$ m)



Characteristic shear rate by droplet impact:

$$\dot{\gamma}^* = \frac{2 \cdot u}{D} \quad \longrightarrow \quad \eta^*$$

For example:

$$u = 5, \dot{\gamma}^* = 2e5, \eta^* = 14 \text{ mPas}$$

 $u = 0.5, \dot{\gamma}^* = 2e4, \eta^* = 30$  mPas

Measured after painting application





Simulation with shear thinning viscosity (D = 50  $\mu$ m, U = 5m/s,  $\sigma$  = 0.025 N/m, h\_film = 60 $\mu$ m)



Comparison of above results, e.g. angle\_static, with that using droplet with a constant viscosity

- Using shear thinning viscosity, angle\_static = 55°
- >  $\eta^* \sim 14$  mPas by the characteristic shear rate ( $\gamma^* = 2e5$  (1/s)), angle\_static = 50°

![](_page_11_Picture_6.jpeg)

Effects of initial positions of flake on the final orientation (h\_film = 60 $\mu$ m,  $\eta$  = 20 mPas )

![](_page_12_Figure_2.jpeg)

- lower angle to horizontal for IniPos. 2&3
- For  $D = 50\mu m$  and a given lacksquarelow viscosity, angle increases with increasing of **Re-Number**
- For large droplets D >= 100µm, situations are complicated
- For spray painting process,  $\bullet$ dominant droplet size < 50 μm

![](_page_12_Picture_7.jpeg)

![](_page_12_Picture_8.jpeg)

# Computational performance

The numerical flow simulations were performed using the commercial flow solver ANSYSFluent v19.5 on the HPE APOLLO (HAWK) of the High Performance Computing Center (HLRS) in Stuttgart. The maximal128 cores/node is suggested to use.

- More memory per core is required because of the dynamic mesh adaption with overset-method
- \* The calculation with 32 cores/node and 256 cores used in total shows a better performance.

![](_page_13_Figure_4.jpeg)

A simulation case with 130 million cells was calculated up to 0.1 - 0.5ms of physical time with time step size < 1e-7s. Using 8 nodes and 256 cores, it consumed about 150 - 760 hours. The latter corresponds to the case with a large droplet.

![](_page_13_Picture_6.jpeg)

#### Summary

A detailed numerical study of the flake orientation by the viscous droplet impact on dry/wet solid surfaces has been carried out.

- A dynamic contact angle model that is suitable to the spray painting process was proposed and validated by the experimental observations
- Implementing a rigid body motion solver for calculating flake movement in ANSYS-Fluent
- A first parameter study was performed
  - Higher liquid viscosity is unfavorable to the flake movement and orientation
  - For real paint liquid, Non-Newtonian behaviors should be taken into account. The proposed characteristic shear rate and the resulting characteristic viscosity can be used to determine the suitable impact velocity
  - For a given low viscosity, small droplets (D = 50µm) with low impact velocity will benefit the final flake orientation without a strong film surface waviness

## Outlook

- Further parameter study for D < 50 µm and 50 < D < 100µm ...</p>
- Flake orientation by baking processes....

![](_page_14_Picture_11.jpeg)

![](_page_14_Picture_12.jpeg)

Thank you very much For your attention

![](_page_15_Picture_1.jpeg)

![](_page_15_Picture_2.jpeg)