

## On a Stochastic Model for a Thermal Spray Coating Process: Prediction of Coating Thickness and Porosity

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### Abstract

In this paper, a 3-D stochastic model is presented to predict the coating thickness and porosity in a thermal spray coating process. The results for different materials are obtained and compared to each other. The model is based on prescribed rules in calculating the splat size during the impact of individual droplets on the substrate. Due to thermal stresses during droplet solidification, the edge of the splats is curled up. This mechanism was assumed to be the sole reason for porosity formation. Simulations are performed for a small section of a substrate on which alumina, aluminum and nickel droplets are sprayed. The computed thickness and porosity was found to be in good agreement with those reported in the literature [1,3].

**Keywords:** Stochastic model, Thermal spray process, Coating porosity, Coating thickness.

### Introduction

Thermal spray coating is a particulate deposition process in which powders of a material are injected into a high temperature flame region where they are melted and propelled towards the surface of a substrate where individual molten particles impact, cool and solidify to form a deposit. This technology is used to produce coatings for wear, thermal, oxidation, and corrosion protection. Extensive theoretical, experimental and numerical studies have been reported in the literature to better control this process. The ultimate goal of research efforts in this field is to establish predictive correlations between the processing parameters and the properties of the coatings. Thermal coating has a stochastic nature. Modeling the buildup of a coating formation from the impact of individual droplets can only be performed using stochastic models less reported in the literature. Cirolini et al. [2] simulated coating deposition with a two dimensional stochastic model without considering the splat curl-up and used a set of complex rules to represent interaction between the splats. Ghafouri-Azar et al. [3] used a Monte-Carlo approach to model 3D coating formation with a normal distribution assumption for spray

parameters. Belashchenko and Chernyak [4] used a stochastic approach to optimize thermal spray coatings. Their modeling results are in reasonable agreement with bond strength test data for the plasma-, arc-, and flame-spray processes as well as wear resistance data for arc-sprayed steel coatings. In this study, we developed a 3D stochastic model based on Poisson distribution for spray process parameters and a new method for simulating the splat curl-up to model the microstructure and thickness of thermal spray coatings.

### Mathematical Model

#### Stochastic model

Four main assumptions used in the model are: the spray droplets are non-interacting point particles; each droplet has a different size, velocity, and impact position; the spray is random; and the probability of obtaining a droplet occurrence at any instant is independent of other droplets occurring at other instants. In the model, dispersed molten droplets on the substrate are generated randomly. It is assumed that the position of impact follows the uniform distribution and the droplet specified diameter and velocity follow Poisson distribution with user specified mean ( $\lambda$ ) and standard deviation ( $\sigma$ ) as:

$$f(s; \lambda) = \frac{e^{-\lambda} \lambda^k}{s!}, \quad [1]$$

$$f_{Poisson}(s; \lambda) \approx f_{normal}(s; \delta = \lambda, \sigma^2 = \lambda)$$

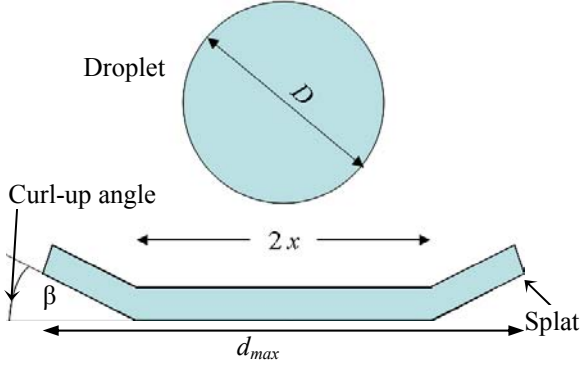
where  $s$  is the stochastic parameter and  $\delta$  is the mean of normal distribution. The Poisson distribution will approach a normal distribution if  $n > 100$  and  $(n \times p) < 10$  where  $n$  is the number of occurrences and  $p$  is the probability of occurrence. A normal distribution has been used by Ghafouri-Azar et al. [3] for velocity and the logarithm of diameter.

To generate random Poisson-distributed numbers for droplet parameters, we used the FORTRAN library written by Ahrens and Dieter [5].

### Model of splat formation

Final splat shapes are sensitive to the spacing between droplet centers, velocity of droplet and temperature of the substrate. These parameters are characterized by dimensionless numbers known as Reynolds (Re), Weber (We) and Stefan (Ste). Droplets diameter, velocity and impact location were introduced randomly as mentioned above. It is assumed that droplets impinge and spread on the substrate one after another.

The developed model includes a set of rules that specify the final splat shape as a function of droplet impact conditions. The model assumes that a spherical droplet with initial diameter  $D$ , after impact on the substrate spreads to form a cylindrical disc of diameter  $d_{max}$  as in Fig. 1. Thus, the effects of any droplet splashing and breakup are neglected.



**Figure 1.** Schematic of the droplet before impact and the formed splat after impact

We used the following relation for spread factor  $\xi_{max}$  derived by Passandideh-Fard et al. [6] based on their experiments and simulations:

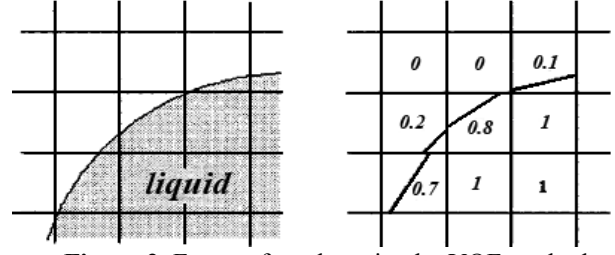
$$\xi_{max} = \frac{d_{max}}{D} = \sqrt{\frac{We + 12}{3(1 - \cos\theta) + 4(We/\sqrt{Re}) + We\sqrt{\frac{3 Ste}{4 Pe}}}} \quad [2]$$

where  $D$  is diameter,  $\theta$  contact angle,  $Pe = Re \cdot Pr$  and

$$Re = \frac{\rho V D}{\mu}, \quad We = \frac{\rho V^2 D}{\gamma}$$

$$Pr = \frac{C_l \mu}{k}, \quad Ste = \frac{C_l (T_m - T_{w,i})}{H_f}$$

in which  $C_L$  is the specific heat,  $T_m$  melting point temperature,  $T_{w,i}$  substrate temperature and  $H_f$  heat of fusion. The numerical methods for driving these relations are based on the energy conservation law. Initial kinetic and potential energy (surface tension) of droplet before impinging on the substrate are dissipated by viscosity after impact. Relation 2 is used by numerous authors like Ghafouri-Azar et al. [3] and Mostaghimi and Chandra [7]. The surface of the coating and the location of pores are determined using a method known as the volume fraction (VOF). In his method a scalar function  $f$  is used for each cell in computational domain. Hence,  $f$  equals unity when the cell is filled with material and zero when the cell is empty. For a partially filled cell we have  $0 < f < 1$  (Fig. 2).



**Figure 2.** Free surface detection by VOF method

### Model of splat curl-up

In this model, it is assumed that solidification starts after spreading the droplet on the substrate and forming the disk shaped splat. Due to temperature difference between splat and substrate, solidification starts from the bottom of splat. Solidification results in thermal stresses that cause the edge of the splat to curl up. This, in turn, is the main source of porosity formation. Curling up at the edge of splats is frequently observed in thermal spray coatings and is one of the main sources of coating porosity. The degree of curling up is affected by several factors, such as stresses generated by mismatch of thermal expansion coefficient at the coating interface, surface tension of the liquid splat, surface roughness, and remelting. Because the mechanism of the curling up is extremely complicated, few attempts have been made to quantify it. In splat curl-up, two parameters are important: one is its starting point and the other is the angle of the curl-up.

Fukanuma [8] proposed a physical and mathematical model for the production of porosity by considering deformation of a molten particle during thermal spray coating processes. He observed that most pores exist at the periphery of splats, starting at around 0.6 times the splat radius ( $R$ ) from the center; this is the criterion used by Ghafouri-Azar et al. [3]. Xue et al. [9] investigated this phenomenon and introduced a simple rule for the amount of splat curl-up as:

$$\beta = \arctan\left(\frac{x R \alpha \Delta T}{h_s}\right) \quad [3]$$

where  $h_s$  is the splat thickness,  $\alpha$  the thermal expansion coefficient,  $R = D/2$ ,  $\Delta T$  the droplet and substrate temperature difference and  $x$  is the starting point of the curl-up (Fig. 1).

### Solution method

After grid generation in the computational domain, the above mentioned stochastic model is used to obtain parameters of each droplet in a random manner. Relation 2 is then used to calculate the splat diameter and VOF method to track the free surface. Having defined the amount of  $x$ , the curl up angle and displacement of splat boundaries are calculated using Relation 3. The cavity formed under the curled up edges are the source of porosity formation. The above procedure continues for each droplet impacting the substrate.

In deposition of droplets on previous splats and coating buildup, the mass conservation algorithm is enforced. The

porosity is defined as the fraction of the total coating volume occupied by voids [3,6]:

$$porosity = \frac{V_g}{V_g + V_m} \times 100$$

where  $V_m$  and  $V_g$  are the volume occupied by solid material and voids respectively.

### Results and Discussion

Coating formation on a small section of a substrate (1mm×1mm) is simulated by spraying 300 alumina droplets with a mean velocity of 100 m/s and a mean diameter of 50  $\mu\text{m}$ . Sample distributions of droplet velocity and diameter are shown in Figs. 3 and 4. First to examine the stochastic model, the program is run several times for the same condition but with different random parameters.

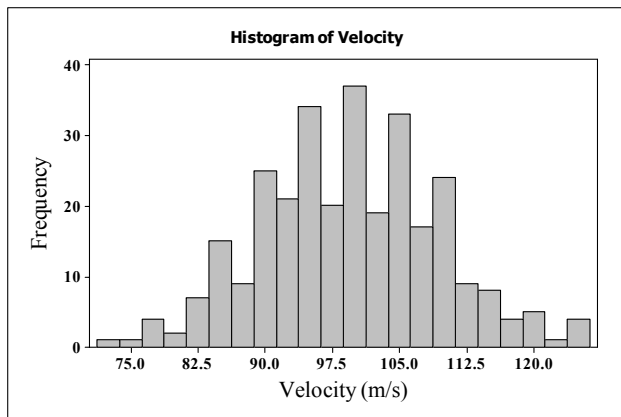


Figure 3: Sample distribution of droplets velocity

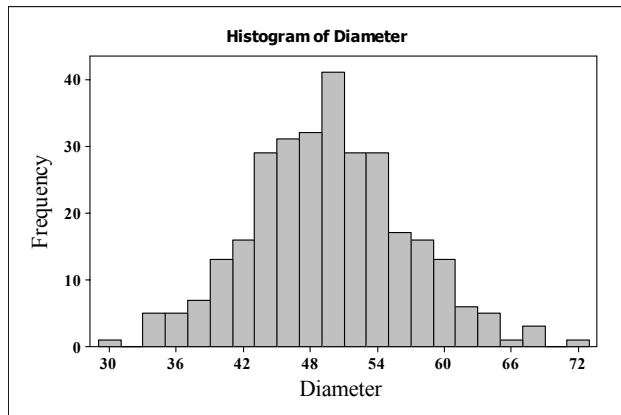


Figure 4: Sample distribution of droplets diameter ( $\mu\text{m}$ )

The results show that despite of different input condition, the results remain nearly the same (porosity is shown in Fig. 5). The obtained average thickness is 14.9171 $\mu\text{m}$  with a standard deviation of 0.4164.

For another thermal spray conditions, the evolution of coating formation is shown in Fig. 6 after deposition of 100, 200 and 300 droplets along with the final surface coating topology. The figure also shows the cross-sectional areas of the final coating. Variation of the coating thickness is shown with color change; pores

within the coating can be clearly seen as holes in the cross sections. The surface roughness is also visible in the figure. The coating formed by impinging 500 Alumina droplets with a mean diameter droplets of 40  $\mu\text{m}$  and a mean velocity of 100 m/s on a steel substrate at 800 K. The program were run for 25 times and the average results were obtained as: porosity=8%, maximum thickness=110  $\mu\text{m}$ , and average thickness=70  $\mu\text{m}$ . For all simulations presented in this paper, the average values of 25 runs with different random parameters were used as the final result.

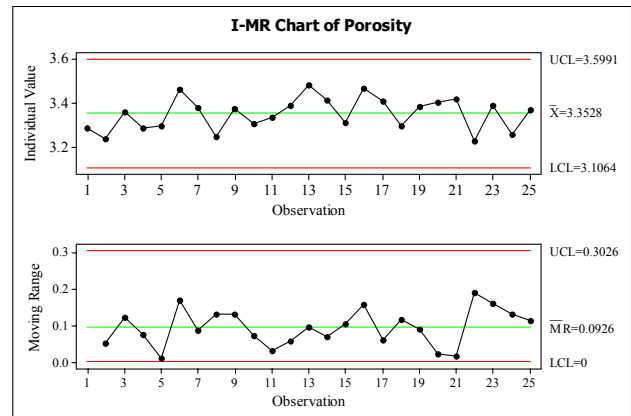
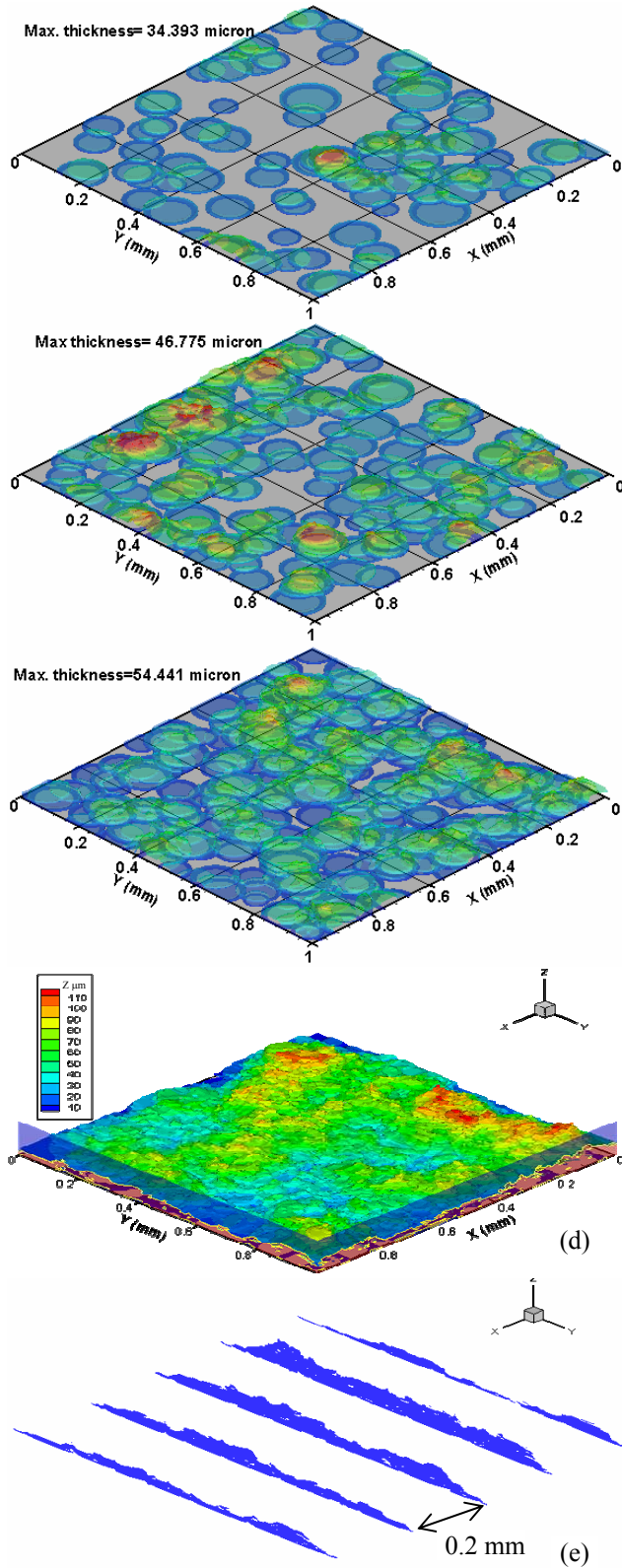


Figure 5: The calculated porosity for 25 runs of the program for one case; the average porosity is 3.3538 with a standard deviation of 0.0734.

In Table 1 the model results are compared with experimental measurements and available numerical results of Ghafouri-Azar et al. [3]. The coating material was nickel. As seen from the table, the model results agree well with those of the Ghafouri-Azar results. In this table the effect of parameter  $x$  is clearly visible. Table 2 shows the comparison between model results with experiments of another reference; again a good agreement is observed. For a substrate temperature of 500 K, the results of the model for droplets of various materials with a mean velocity=100 m/s and mean diameter=50 $\mu\text{m}$ , are compared to each other (see Fig. 7). The amount of  $x$  is assumed to be constant for all cases. Therefore, the difference of the porosity values for different materials can be attributed to droplet physical properties namely the surface tension and liquid phase viscosity.

### Conclusion

In this paper, a thermal spray coating process with various spray materials is simulated using a stochastic model. It is assumed that the splat curl is the sole reason for formation of porosity. Although parameters like thermal contact resistance, oxidation and roughness are not considered in this study, the results are in good agreement with other numerical and experimental results. Simulations are performed for a small section of a substrate on which alumina, aluminum and nickel droplets are sprayed. The computed thickness and porosity was found to be in good agreement with those reported in the literature.



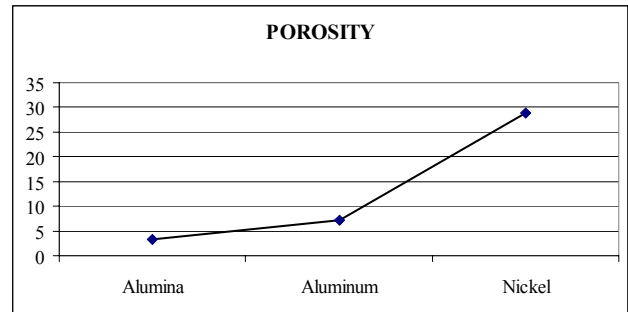
**Figure 6:** The evolution of coating formation from deposition of (from the top) 100, 200, 300 droplets along with the final surface coating topology and several cross sections. The final porosity obtained was 7%.

**Table 1:** Comparison of model predictions with other experimental and numerical results for Nickel

	Exp.	Numerical results		Ghafouri-azar [3]	Numerical results
Mean Diameter ( $\mu\text{m}$ )	43	43		58	58
Mean velocity (m/s)	62	62		60	60
Porosity%	7.7	6.68	13.92	11.1	11.83
Average Thickness (mm)	-	0.169	0.196	0.4224	0.4574
$x$		0.75	0.6	----	0.75

**Table 2:** Comparison of model predictions with other experimental and numerical results for Alumina

	Pawlowski [1]	Present paper
Material	Alumina	Alumina
Mean Diameter ( $\mu\text{m}$ )	-63+16	63
Mean velocity (m/s)	125	125
Porosity%	6.8	7.23
Average Thickness (mm)	----	0.0557
$x$	---	0.6



**Figure 7:** The effect of spray droplet materials on the porosity of the formed coating

### Nomenclature

$C_L$	liquid specific heat
$D$	particle diameter
$d_{max}$	splat diameter (assumed to be disk shaped)
$f$	liquid volume fraction function
$H_f$	heat of fusion
$h_s$	splat thickness
Pe	Peclet Number
$R=D/2$	splat radius
Re	Reynolds number
$s$	stochastic parameter
$T_m$	melting point temperature
$T_{w,i}$	substrate temperature
$V$	particle velocity
$V_m$	volume occupied by solid material
$V_g$	volume occupied by voids
We	Weber number

$x$	starting point of the curl-up
$\alpha$	thermal expansion coefficient
$\beta$	curl-up angle
$\gamma$	surface tension of the droplet
$\delta$	mean of the normal distribution
$\theta$	contact angle at the droplet/substrate contact line
$\mu$	molten particle viscosity
$\rho$	particle specific mass
$\xi_{\max}$	flattening degree
$\Delta T$	droplet and substrate temperature difference

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