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A machine learning approach for adhesion forecasting of cold-sprayed coatings on polymer-based substrates

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Abstract. Cold spray is a novel production technology for creating metallic layers on various materials. Using a pressurized gas travelling at supersonic speeds, the metallic particles are accelerated and impact the target surface obtaining adhesion through mechanical interlocking between the powders and the substrate. This method is especially well suited for coating thermosensitive materials like composites since it only requires a little amount of heat, as the powders remain in a solid state. The quality and comprehension of this manufacturing process can be greatly improved by using machine learning techniques. In order to evaluate the characteristics of the particle's deformation upon collision, the goal of this work is to forecast it using machine learning approaches. The parameters chosen as an input for the model were related to 3 macro-categories: process parameters, powder parameters and substrate parameters. As regards the output parameters, flattening and penetration were chosen as they are the main characteristics of the coating on which homogeneity and adhesion depend. In order to obtain reliable results, a mix of data FEM and experimental data were used to train the neural network. The model was then tested on a dataset of experimental data.

Introduction

The drive to reduce weight and manufacturing costs has raised the demand for polymeric materials dramatically in recent years. Thermosetting polymers, in particular, have become widely employed in a variety of industries, including aerospace, since they may be used as matrix for fibre-reinforced composite materials. However, as environmental concerns become more generally acknowledged, the use of thermosets is severely limited since they cannot be reused or recycled once the curing process is complete. High-performance thermoplastic materials, such as PEEK or ABS, are gaining popularity because of their high toughness, high melting temperature, and 100% recyclable nature.

Nonetheless, several applications remain out of reach because of these materials' poor surface qualities, such as poor wear and scratch resistance and low electrical conductivity. As a result, surface metallization may be the best option for combining the benefits of metals with thermoplastic polymers. However, when using the most common metallisation procedures, the melting temperature of the metallic materials to be sprayed must be reached, modifying its original properties and causing thermal distortions in the substrate.

Cold Gas Dynamic Spray, which uses kinetic energy and involves temperatures well below the melting point of the metallic particles, can be an adequate alternative for improving the surface properties of polymers [1].

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This approach is based on the high-speed impact of solid-state metallic particles; no chemical reactions are required, and deposition is made possible in large part by mechanical interlocking between the particles and the substrate [2].

Although this technology has been widely explored and employed on metal substrates, the underlying physics when the substrate is a polymer is yet unclear [3]. Because the final coating characteristics (such as powder deformation or penetration depth, which are closely related to coating adhesion) depend on a variety of factors, including the properties of the metallic powder and the polymeric substrates, as well as the spraying parameters set for the process, it is currently impossible to accurately predict how the metallic particles will behave when they impact on various substrates.

For this reason, several computer models have been developed recently to mimic the Cold Spray process' operational parameters and predict how a particle would behave when it comes in touch with a substrate [4-6]. The coating process utilized on polymers and composites, however, has only been the subject of a small number of publications published so far. A physical model that could precisely depict the processes that occurred when metallic particles were deposited on non-metallic substrates, however, was not practical to develop. In order to validate those models, it would be necessary to gather hundreds of testing scenarios and outcomes utilizing top-of-the-line tools (including sensors and high-speed cameras).

In this scenario, machine learning might potentially reduce the number of required experimental trials. As machine learning (ML) solutions are typically considered "black boxes," in order to have accurate forecasts, it is necessary to feed the model with accurate and numerous data. For this reason, training the model with a mix of experimental data, which are accurate but often scarce and fragmented, and computational data obtained from Finite Element models (FEM), which do not suffer from the issues of experimental data but are less accurate, could be a good solution to obtain accurate predictions of the coating characteristics.

With knowledge of the process parameters, particles and substrate characteristics, a machine-learning approach is used to forecast the deformation and flattening of the metallic particles after deposition.

Using low-pressure equipment, 30% of the data from the training set and the entire test set were collected experimentally, employing SEM analyses to determine the flattening and penetration depth.

The remaining test dataset was produced by performing a FE simulation of copper, aluminium, steel and particles collision upon PEEK and ABS-based polymeric substrates. Three best Machine Learning models have been selected: Linear regression, Gaussian process regression and Neural networks. In order to provide a methodological approach for future studies, a comparison of the results obtained with a dataset entirely composed of data obtained from the FE model and of the results obtained with the dataset composed of a mix of experimental and FEM data is proposed.

Materials and Methodologies

Input and output parameters**.**

The input parameters for the employed strategies fall into three macro-categories: impact velocity, which includes all the other process parameters such as temperature and pressure; *powder parameters* (Yp), which represent the yield strength of the powder material and *parameters of the substrate* (Ys), i.e. the yield strength of the substrate material, which also takes into account the presence of the fibres since these, if positioned appropriately under a layer of matrix at least comparable to the size of the powders, only stiffen the substrate, thereby causing a variation of the yield strength. The considered output parameters are the *penetration depth* of the particle and the *flattening*. The definition and evaluation of both parameters is furtherly illustrated in the following sections.

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Dataset.

As highlighted in the introduction, the datasets employed were constructed employing both FEM and experimental data. In particular, the first training dataset is composed of 30% experimental data and 70% FEM data (mixed data), while the second dataset contains only FEM data. The test dataset for both suggested models is fully made up of experimental data.

CS experimental input data generation.

The substrate selected for the deposition was Polyether-ether-ketone (PEEK) and Acrylonitrile butadiene styrene (ABS), both unreinforced and reinforced with long carbon fibres.

The copper, aluminium and steel spherical powders were provided by LPW South Europe. Low-pressure cold spray equipment (DYCOMET) was used to conduct the aforementioned depositions.

Air was used as the carrier gas since earlier research found no discernible changes when other carrier gases were used [7–9]. The samples were positioned on a platform, and the spraying gun was installed on a robot (HIGH-Z S-400/T-CNC-Technik) and operated remotely while operating perpendicular to the substrates. The process parameters employed and the characteristics of the powders employed for the experiments are highlighted in Table 1.

Table 1. Characteristics of the powders and process parameters employed for the CS experiments.

Particle parameters	***Copper***	***Aluminium***	***Steel***
Mean radius [μm]	20	18	23
Yield strength (Yp) [GPa]	0.033	0.18	0.29
Process parameters			
Inlet Gas temperature [°C]	100 - 400	100 - 400	100 - 400
Standoff distance [mm]	10 - 4	10 - 4	10 - 4
Inlet gas pressure [MPa]	0.5 - 0.6	0.5 - 0.6	0.5 - 0.6
Gun traverse speed [mm s^{-1}]	7.5	7.5	7.5

For the purpose of measuring the flattening of the powders, the top surface of the coating was examined. The mean radius of the particles after the collision with the substrate (r) was measured using Image J software to calculate the percentage of particle flattening, defined as $r/r_0\ [\%] = \frac{(r-r0)}{r0}100$, where r_0 is the mean radius of the particle before the impact. The flattening values taken into account are the average flattening values calculated on three separate 500x500 micron micrographs that were examined. In order to evaluate the radius before and after the impact, SEM micrographs were analyzed through the Image J software, as portrayed in Fig.1.

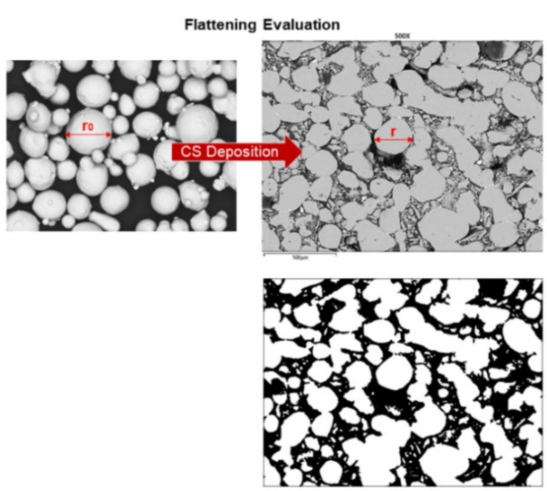

Fig. 1. Evaluation of the particles' mean radius before (r_0) and after the deposition (r).

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To measure the penetration depth, the specimens were cut perpendicular`r to the top surface to inspect the cross-section and evaluate the height of the particle upon the impact [Hs0]. The penetration depth was defined as $Hs\,[\%] = \frac{(Hs_0 - Hs)}{Hs}\,100$. The specimen cross section was analysed in order to evaluate the height of the particle after the impact, SEM microscopy was employed as shown in Fig 2.

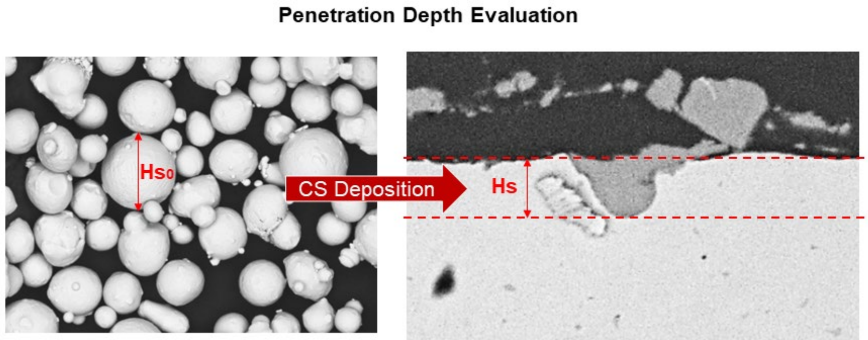

Fig. 2. Evaluation of the particles' mean height before (Hs_0) and after the deposition (Hs).

FEM input data generation.

A Lagrangian reference frame, which is frequently utilized in literature to represent high-velocity impact with minimal computing expense, was employed to model both the particle and the substrate. Using a 2D-axisymmetric model and an explicit dynamic analysis that took into account adiabatic heating effects, it was possible to simulate a spherical particle hitting perpendicular to a substrate that is at least five times bigger than the particle. This particle-to-substrate size ratio was determined by assuming that the elastic waves reflected from the boundaries did not reach the interface upon impact.

In keeping with the average particle size of the powder utilized for the experimental tests, a particle diameter of 20 microns was used for the simulation. The features of the substrate and the particles have been identified via earlier experiments using the supplies on hand at the testing site.

The Johnson-Cook model for plastic materials was used to model the behaviour of both the particle and the substrate's materials, and one of the ABAQUS software's algorithms—the surface-to-surface penalty contact algorithm—was used to model the interaction between the substrate and the impacting particle. The impact simulations were performed for each material combination (copper, aluminium, 316L steel, on PEEK and ABS) by varying the particle's speed between 50 m/s and 350 m/s with an increasing step of 30 m/s. The model generated 50 different values for the particle's penetration and flattening ratio depending on the input parameters.

ML Approaches and Performance Evaluation

We used three machine learning approaches: Linear regression (LR) Gaussian process regression (GPR) and Neural networks (NNs). LR is a simple method for determining a linear relationship between variables. This relationship illustrates the functional connection between the independent and dependent variables for a specific dataset. Consequently, LR models the unknown or dependent variable and the known or independent variable as a linear equation [10].

GPR is a nonparametric Bayesian method used for regression [11]. It performs well on small datasets and it infers a probability distribution model over all acceptable data-fitting functions. The neural network employed is a function-fitting neural network with three layers which is trained on the whole dataset. It can generalize an input-output relationship after training the data.

In order to evaluate the performance of the ML approaches, we calculated the Root-mean-square error (RMSE) [11], the R-Squared [12], the Mean Squared Error (MSE) [13] and Mean Average Error (MAE) [14].

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RMSE is the square root of the squared mean error and is an outlier-sensitive metric.

R-squared is a linear regression model goodness-of-fit metric which represents the proportion of the variance in the dependent variable explained by the independent variables. R-squared measures the strength of the association between the model and the dependent variable.

The MSE indicates the mean squared discrepancy between the observed data values and the estimated data values.

MAE represents the distance between the predicted value and the measured value. When the values of these metrics are low, the model is more accurate.

Results and Discussion

In this section, the experimental results on the FEM dataset and the mixed dataset (FEM and experimental data) will be shown and discussed. Below are the best findings from each experiment.

Experiments with FEM-based dataset.

Observing the output by training the model with FEM data, it was possible to assess that the best models on the test set for penetration and flattening prediction were the forecast obtained with the GPR method (see Fig.3 and Fig.4). More specifically, the GPR model shows improved the penetration values and a decline in flattening performance. To comprehend this decline in flattening model evaluation metrics, further studies need to be conducted.

Penetration depth prediction (GPR)	
RMSE	1.45
R-Squared	0.73
MSE	2.1026
MAE	0.7654
Prediction Speed	~2200obs\sec

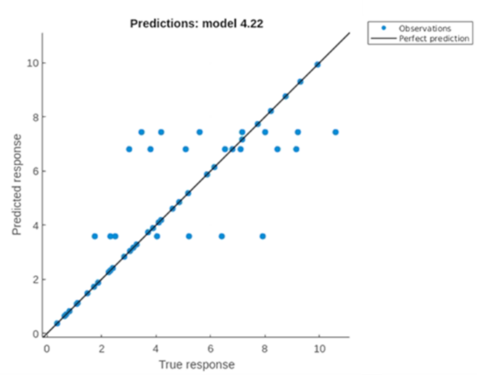

Fig. 3. Performance for the penetration depth prediction for FEM data.

Flattening prediction (GPR)	
RMSE	4.7387
R-Squared	0.34
MSE	22.451
MAE	2.0051
Prediction Speed	~1900obs\sec

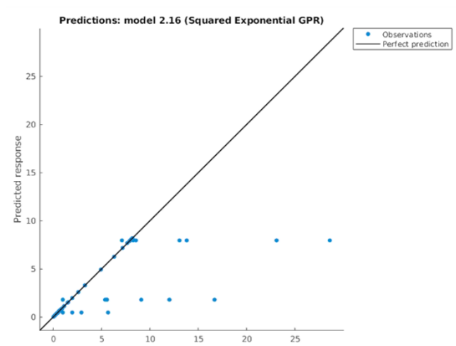

Fig. 4. Performance for the flattening prediction for FEM data.

Since the error values are quite small, we may conclude that the FEM models are capable of approximating the experimental data fairly correctly. In this context, machine learning can be an excellent tool for accelerating finite element analyses, which require a high computing cost. For this reason, machine learning may be used to simplify the models without losing information or to perform predictions on additional combinations of materials without the need to run additional simulations.

Experiments with dataset MIX.

The top models for the penetration on the test set are NN and LR for the flattening prediction, according to training the model with mixed data, as we can see in Fig. 5 and Fig. 6.

Penetration depth prediction (NN)

RMSE	0.5842
R-Squared	0.96
MSE	0.3413
MAE	0.413
Prediction Speed	~400obs\sec

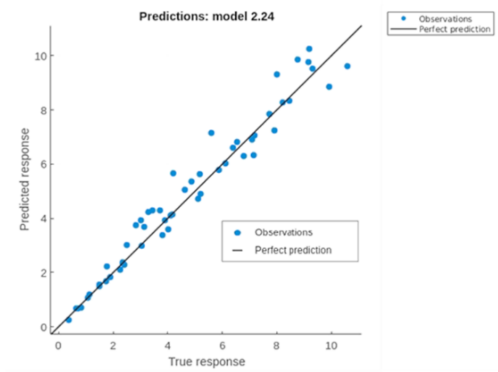

Fig. 5. Performance for the penetration depth prediction for mixed data.

Flattening prediction (LR)

RMSE	1.8327
R-Squared	0.90
MSE	3.3587
MAE	1.4462
Prediction Speed	~3800obs\sec

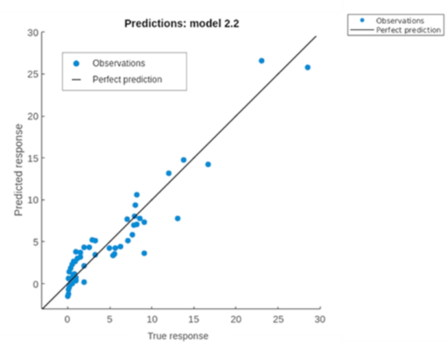

Fig. 6. Performance for the flattening prediction for mixed data.

It is possible to observe that by integrating the training set with experimental data, the prediction error may be furtherly lowered. In fact, by including 30% of experimental data in the training dataset, it is possible to obtain more accurate models.

Future investigations are required in order to assess the optimal value of the ratio between the experimental data and the FEM data in the training set, in terms of the accuracy of the prediction and the resources employed to create the dataset. In Fig. 7, we depicted the comparison of performance for penetration and flattening. For penetration, the best results, except for R-Squared, are achieved when the models is trained with mixed data. A similar behaviour is also evident when we consider the flattening output parameter.

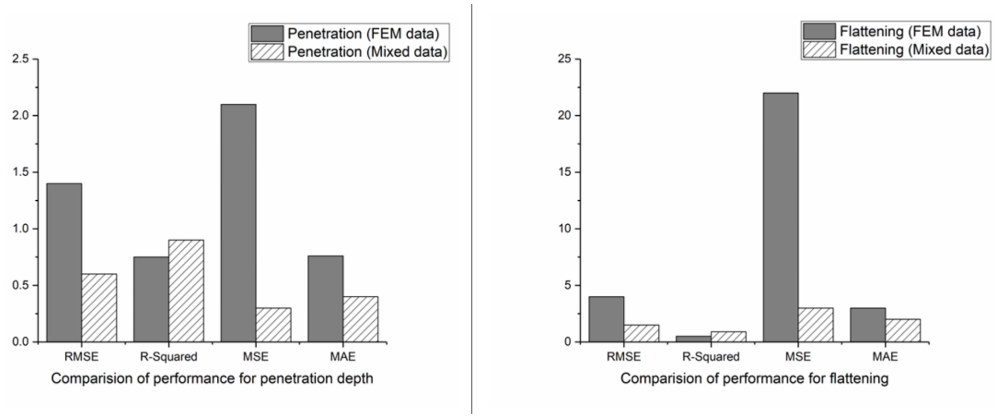

Fig. 7. Performance for penetration and flattening prediction for FEM and mixed data.

Summary

This study provides an overview of how machine learning techniques can be used to more accurately predict particular coating features, such penetration and flattening, in order to increase process efficiency. To be more precise, two sets of data, FEM data and mixed data (experimental and FEM data), were used to test various models, and the best ones—the GPR, LR, and NN—were selected.

The performed experiments show that the models get more accurate as the amount of data available increases. In particular, models fit the data better when trained on the mixed dataset. By providing a preliminary examination of the contribution of the parameters influencing the coating deposition, the use of machine learning appears to contribute to the optimization of the Cold Spray process. Future research can assist expand the dataset required to train the models and forecast the ideal combinations of parameters which will enhance the coating process.

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