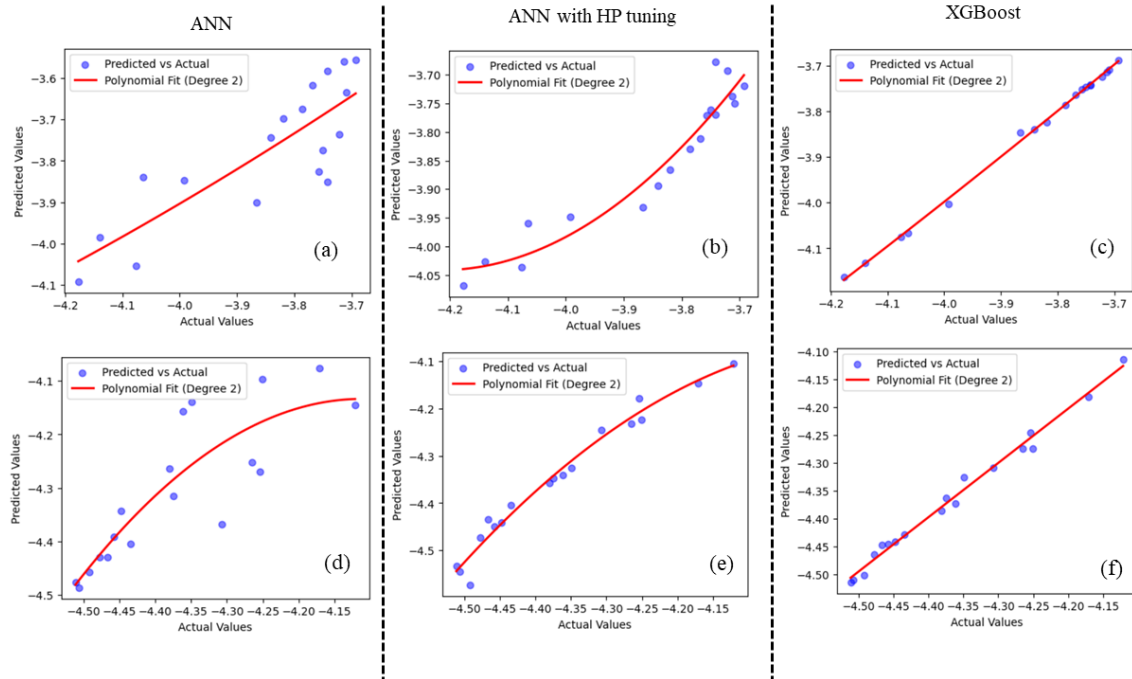


## Surrogate Model-Assisted Machine Learning Optimization of Aerospace Coating Deposition Processes for Enhanced Performance and Uniformity



**Fig. S1** Prediction capability of different ML models (a), (b) & (c) Deposition rate for ANN, ANN with HP tuning and XGBoost models respectively and (d), (e) & (f) Film uniformity for ANN, ANN with HP tuning and XGBoost models respectively

**Table S1** Performance metrics of the different ML models

Model		Deposition rate			Film Uniformity		
		R <sup>2</sup> score	MSE	MAE	R <sup>2</sup> score	MSE	MAE
ANN	Training	0.734	0.0068	0.0695	0.828	0.0065	0.0613
	Validation	0.567	0.0089	0.0767	0.487	0.0015	0.0808
	Test	0.424	0.0142	0.1051	0.311	0.0090	0.0738
ANN with HP tuning	Training	0.903	0.0024	0.0414	0.966	0.0013	0.0279
	Validation	0.872	0.0026	0.0394	0.956	0.0010	0.0248
	Test	0.862	0.0034	0.0499	0.894	0.0014	0.0308
XG Boost	Training	0.999	0.000018	0.00321	0.999	0.000003	0.00048
	Validation	0.996	0.000086	0.00581	0.987	0.000028	0.01103
	Test	0.998	0.000051	0.00479	0.989	0.000014	0.01012

**Table S2** Comparison of error percentage of different ML models with the existing RSM model

Model	% Error			
	Deposition rate		Film Uniformity	
	OPE	Max Error	OPE	Max Error
ANN	1.869	4.667	0.657	4.013
ANN with HP tuning	0.172	2.892	0.437	3.297
XGBoost	0.080	1.756	0.365	2.502

$$\text{OPE} = \frac{\sum_{i=1}^n |y_{pred} - y_{actual}|}{\sum_{i=1}^n y_{actual}} \times 100$$

Where,

OPE – Overall Percentage Error

$Y_{actual}$  – CFD value.

$y_{pred}$  – Predicted value

n number of samples/Data points