Leveraging ML for Predicting Particle Impact Conditions & Bonding in CSAM

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Introduction

~~**Fossil Fuels**~~

- ~~Greenhouse gas emissions~~
- ~~Non-renewable~~

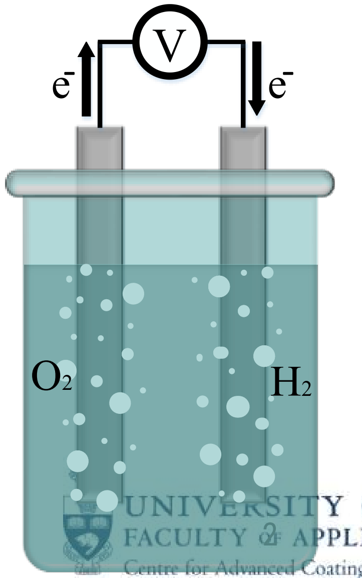
Hydrogen

- No pollution problems
- No intermittently availability problems

One of the most promising hydrogen production techniques:

<u>Alkaline Water Electrolysis</u>

☹ High electricity consumption



Nickel-Based Electrodes

Improve the energy efficiency of water eletrolysis → Reduce the reaction over-potential

→ Intrinsically active electrode materials

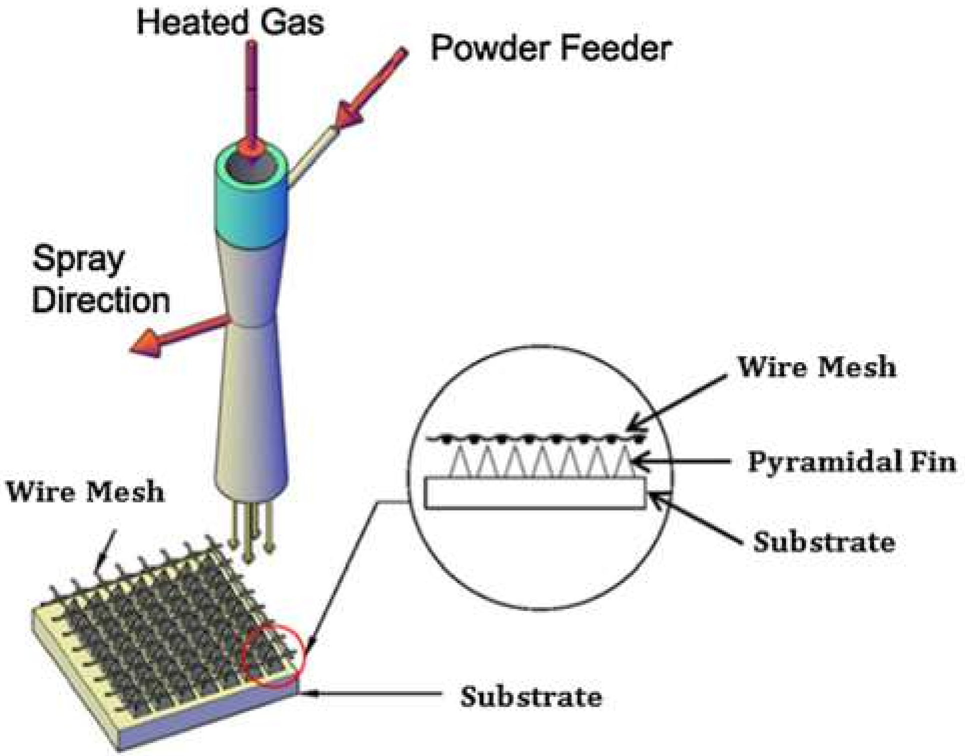
→ Enhancement of the active surface area

Nanocrystalline Catalysts:

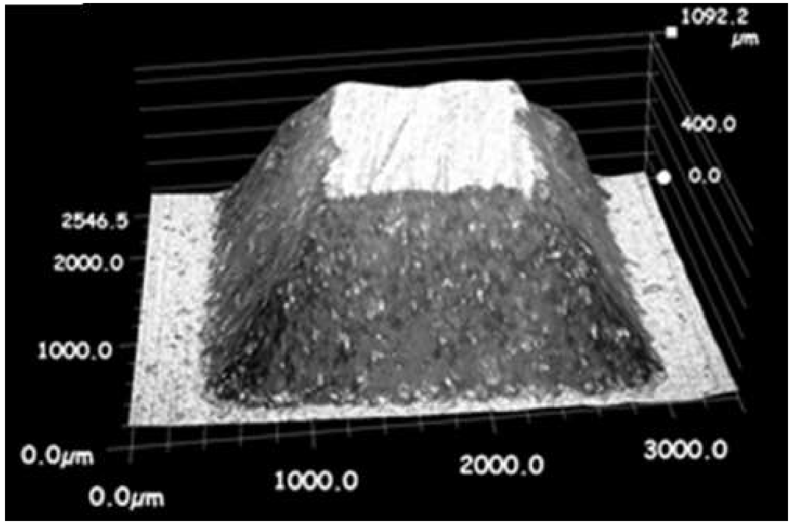
- Increased amounts of atoms located at interfaces between adjacent grains
- Random atomic distances and densities

Masked CS fin production technique

- In the cold spray process, pin fin geometries can be generated by using a mask (e.g., wire mesh)
- The mask is located between the nozzle exit and substrate surface



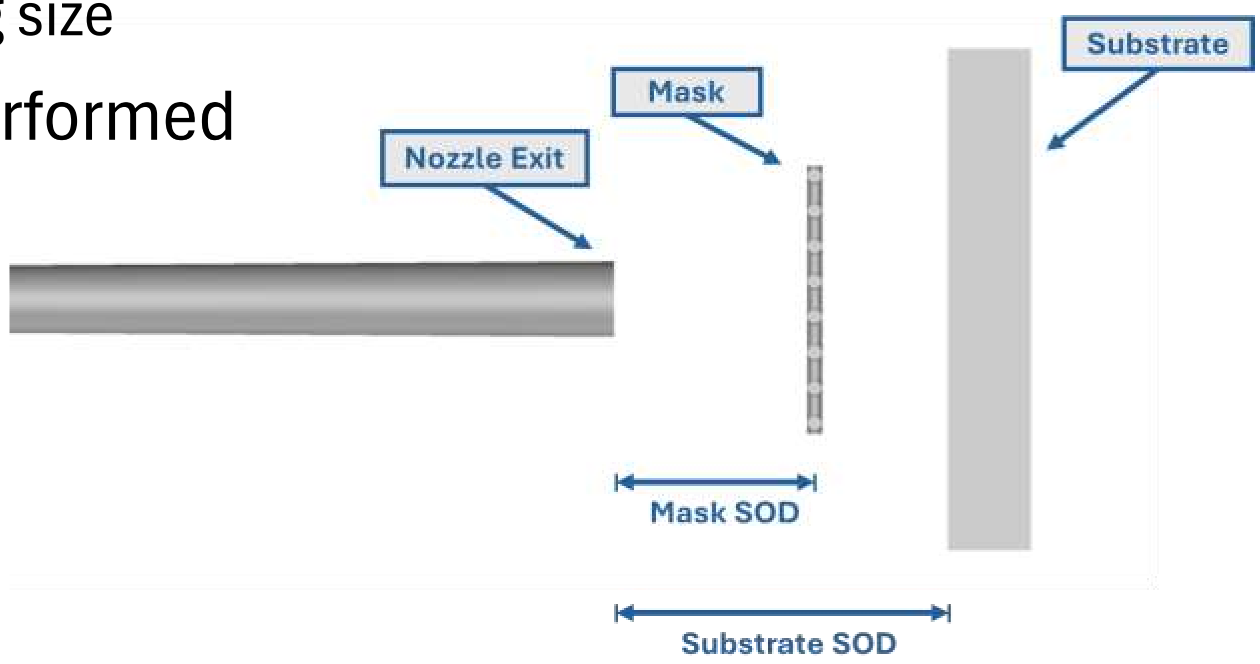
Cormier, Y., Dupuis, P., Jodoin, B. et al. J Therm Spray Tech 24, 476–488 (2015).



Dupuis, P., Cormier, Y., Fenech, M., Jodoin, B. Int J Heat Mass Transfer 98, 650-661 (2016).

CFD simulations

- A parametric analysis was performed to analyze the effect of:
  1. Nozzle inlet operating condition (pressure and temperature)
  2. Substrate standoff distance (SOD)
  3. Mask standoff distance
  4. Mask wire diameter and opening size
- A total of 48 simulations were performed



Mask and substrate SOD identification.

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Study Parameters

1. Nozzle inlet operating condition

- Two operating conditions were analyzed:

Case	***Inlet Pressure (MPa)***	***Inlet Temperature (°C)***
Medium Pressure	2	400
High Pressure	4	800

2 & 3. Substrate and Mask SOD

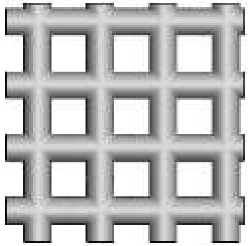
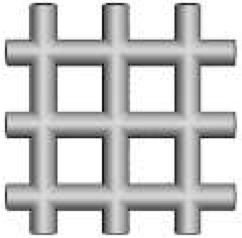
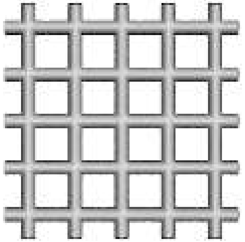
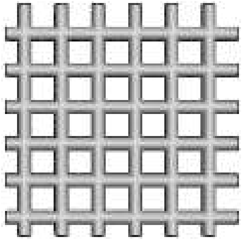
- Two substrate SODs were analyzed (10 and 20 mm)
- The mask SOD was increased at 4 mm increments

	10 mm Substrate SOD *(from Nozzle Exit to Substrate)*	***20 mm Substrate SOD*** *(from Nozzle Exit to Substrate)*
Mask SOD *(from Nozzle Exit to Mask)*	4 mm	4 mm
	8 mm	8 mm
		12 mm
		16 mm

Study Parameters

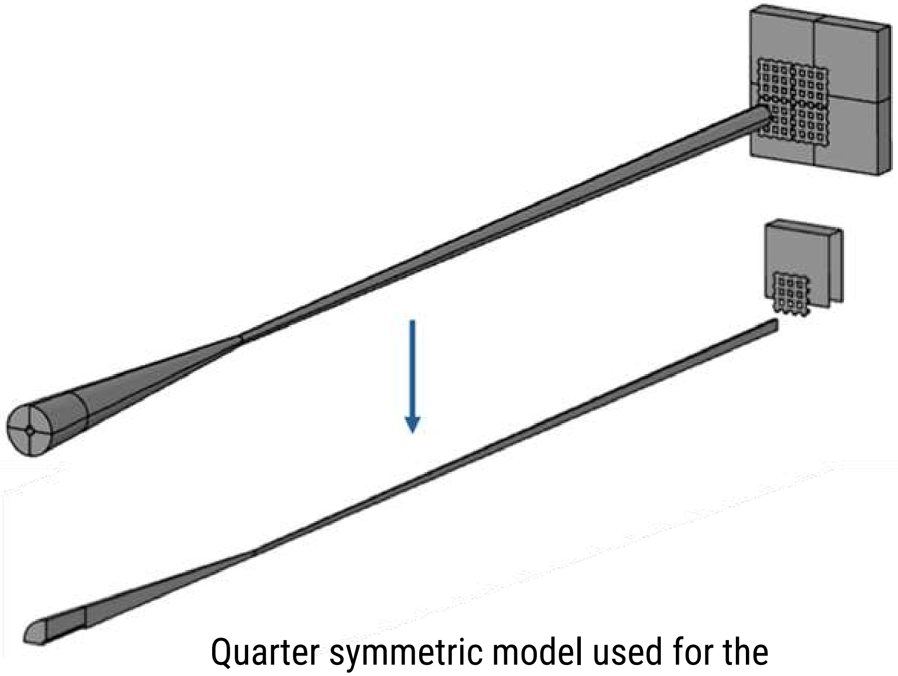
4. Mask wire diameter and opening size

- Two mask wire diameters were analyzed (a small and large diameter)

	Mask 1	Mask 2	Mask 3	Mask 4
Wire Diameter (mm)	0.89	0.89	0.46	0.46
Opening Size (mm)	1.22	1.65	1.14	0.81
% Open Area	33	42	51	41
Model				

CFD simulations

- To model the analysis, a 2-way coupled Eulerian-Lagrangian approach was used
- Since the flow and overall particle deposition is symmetric about two planes, a quarter symmetric model was implemented



Quarter symmetric model used for the analysis.

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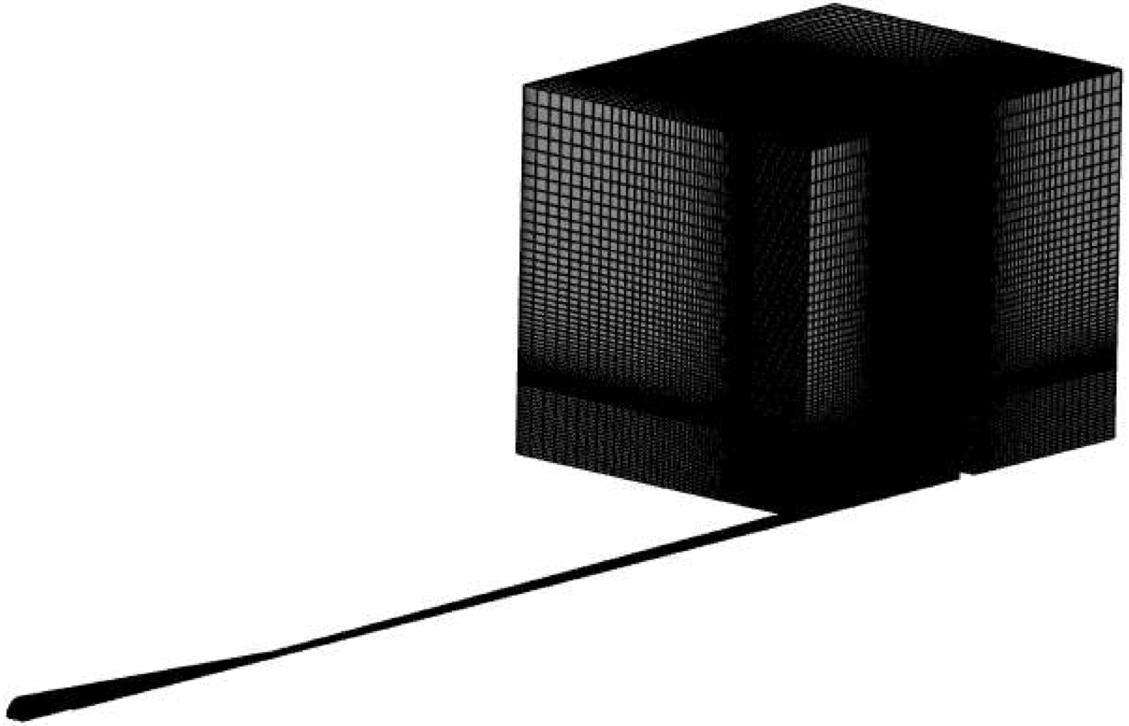
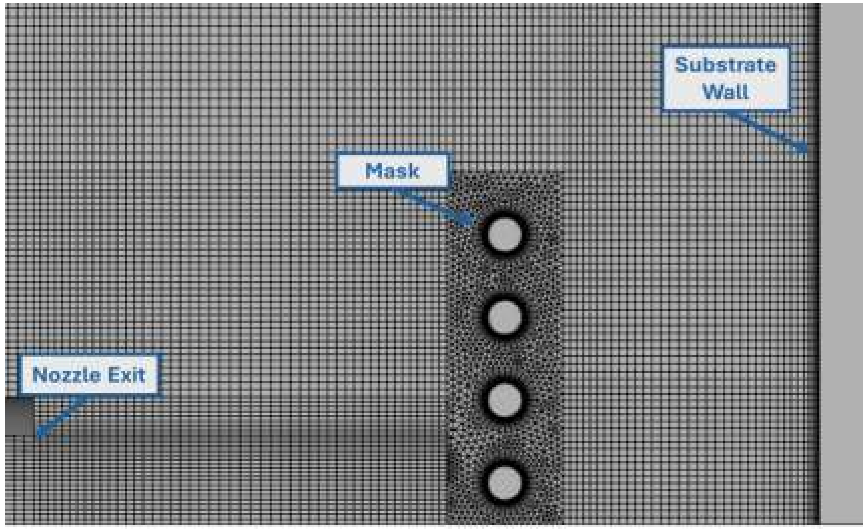
CFD Modelling: Mesh

- The mesh consisted of 1,500,000 to 2,600,000 cells (depending on the mask analyzed and SODs)





Zoomed-in view of the mesh, showing structured and unstructured regions.

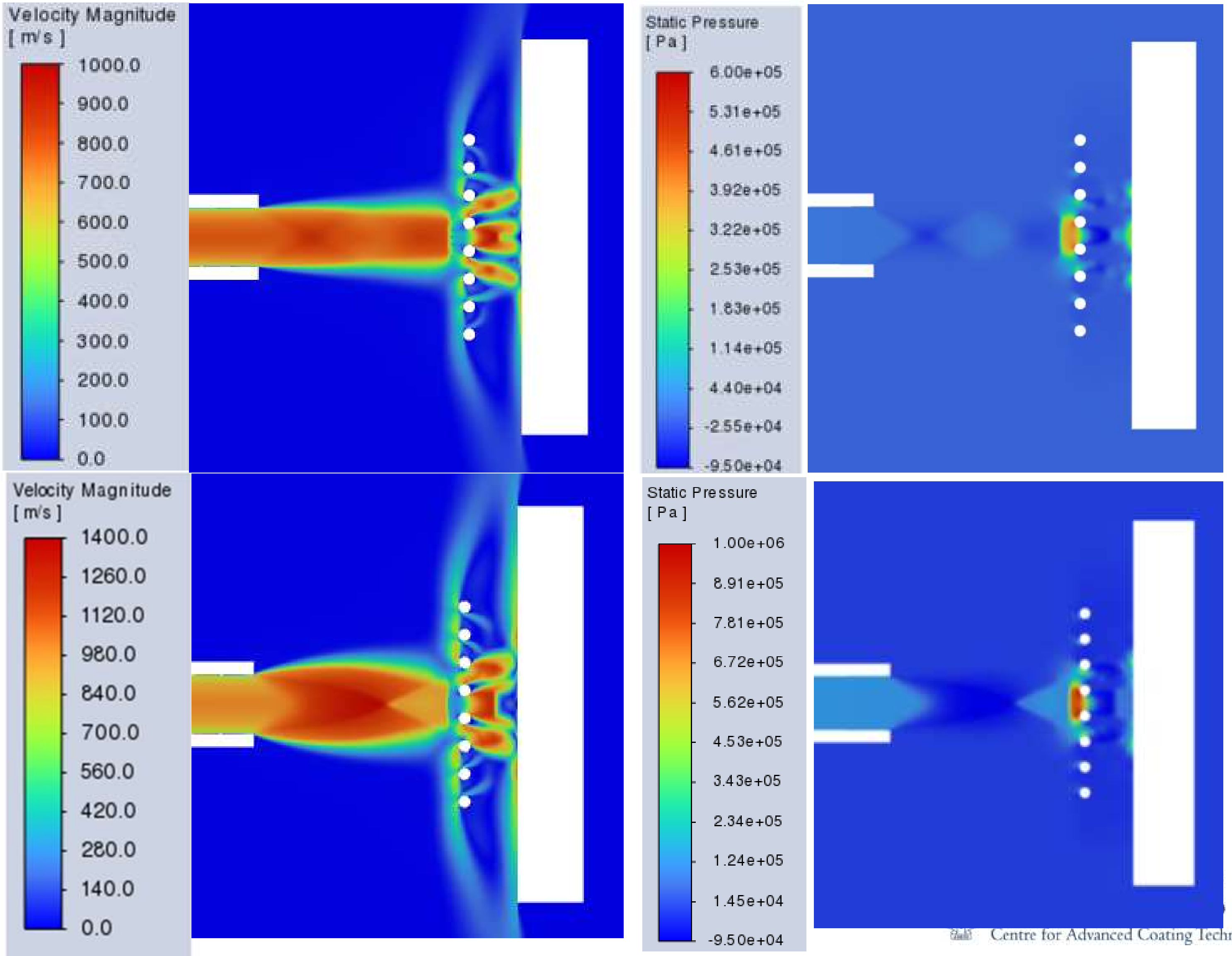
CFD Results: Gas Flow

Effect of inlet pressure

Mask 1, 20 mm substrate SOD, 16 mm mask SOD

Medium-pressure

High-pressure



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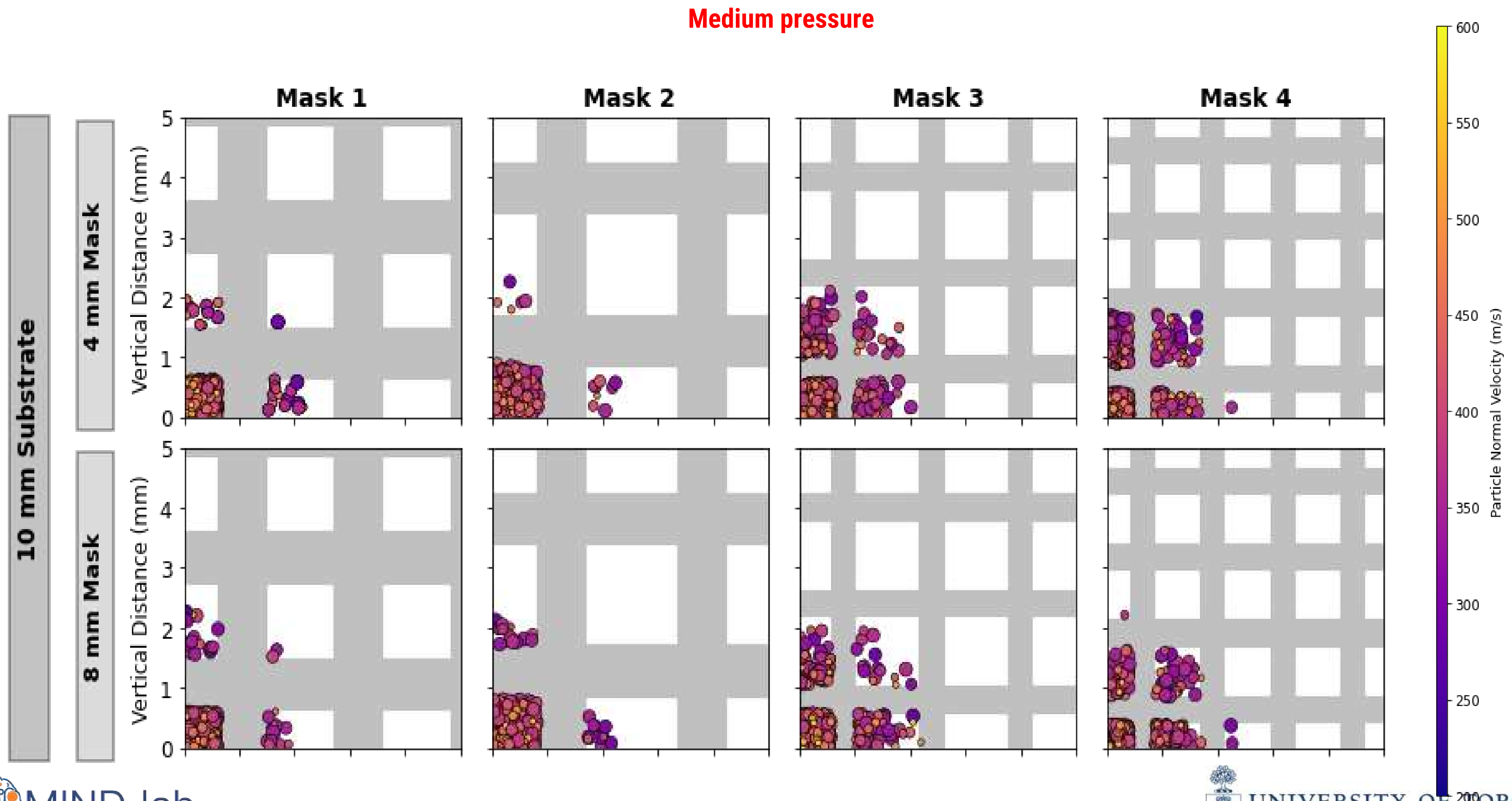
CFD Results: Particle Normal Velocity



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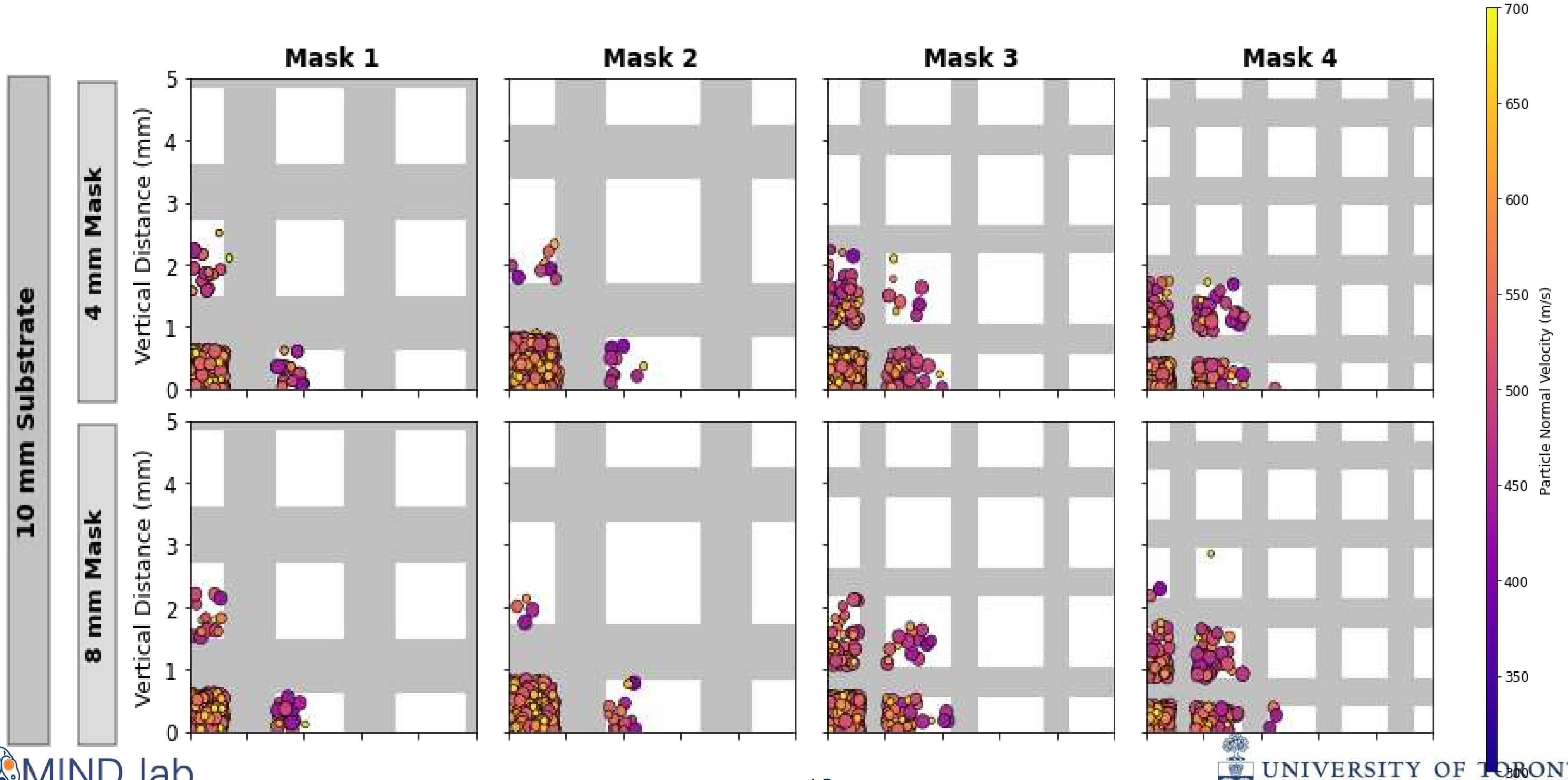
CFD Results: Particle Normal Velocity

High pressure



CFD — Challenges Faced, Insights Gained

CFD is accurate but slow. One detailed run with millions of mesh cells can take hours or even days on a strong computer.

Needs lots of work for generating the geometry and meshing

Turning CFD's heavy grind into lightning-fast, one-click answers—feed the data, unleash the predictor!

Necessary for digital twins

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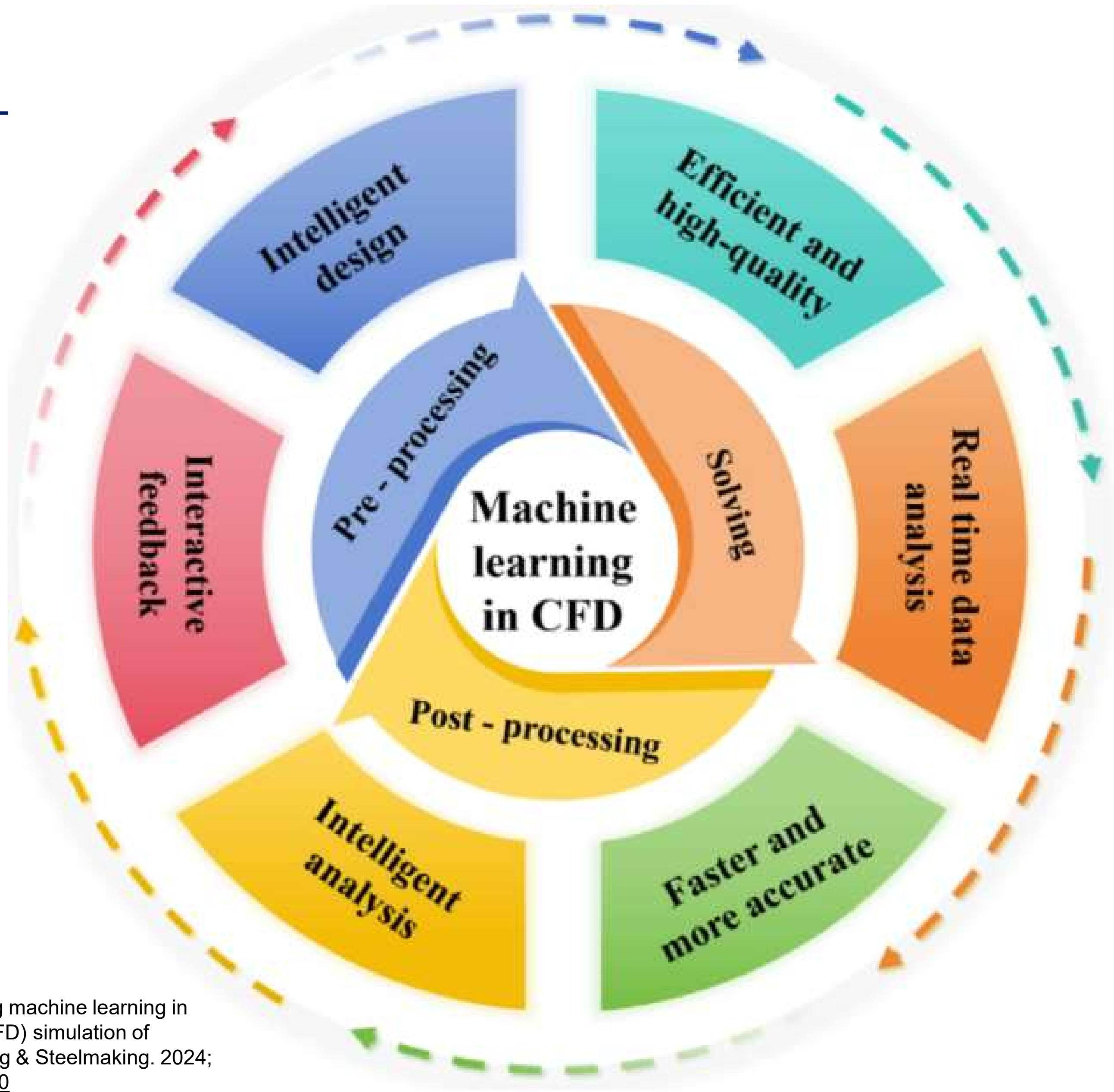
Why ML?

1. significantly **reduce computational costs** while maintaining high predictive fidelity.

2. a step toward creating **real-time digital twins for cold spray systems**.

3. accurately capture the **localized distributions of particle positions, velocities, and temperatures in masked cold spray processes**
   - offering a significant improvement over **traditional ML models that primarily predict average values**



Liu et al. Prospective on applying machine learning in computational fluid dynamics (CFD) simulation of metallurgical reactors. Ironmaking & Steelmaking. 2024; doi:10.1177/03019233241278460

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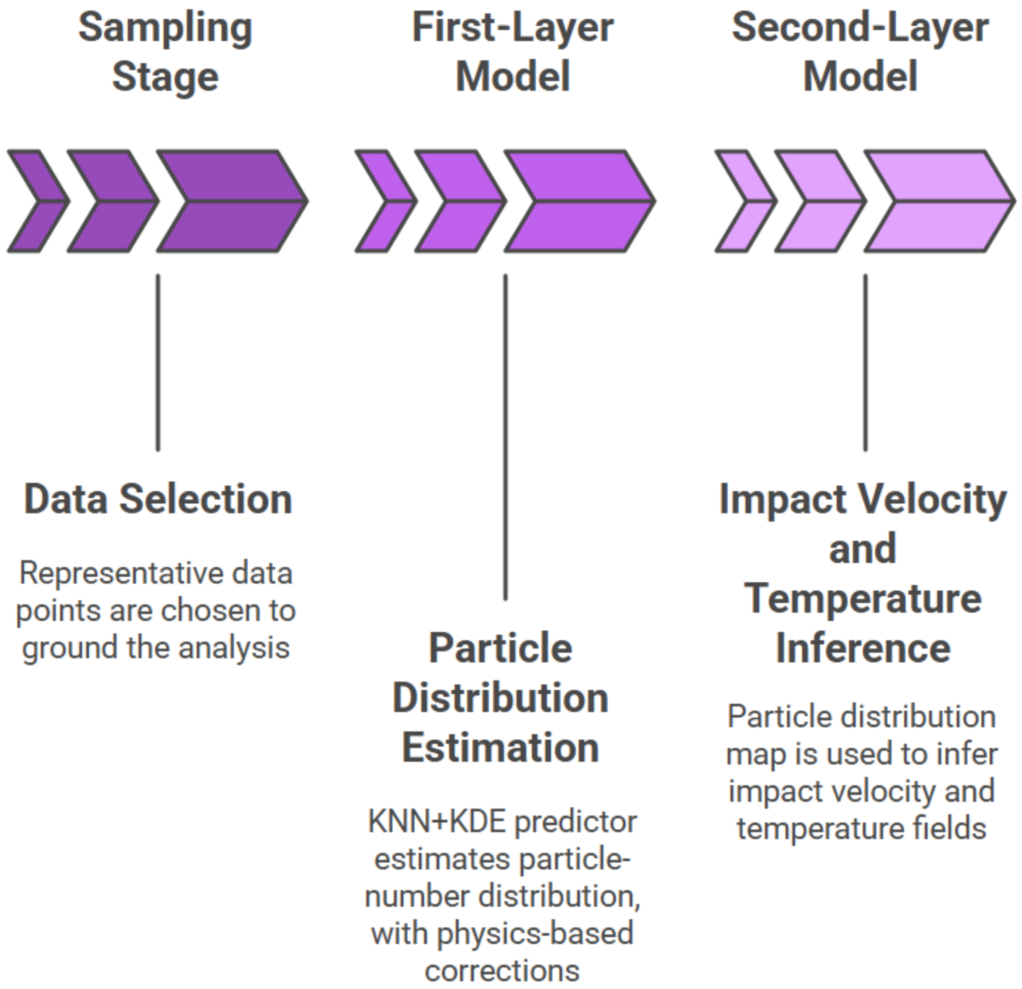
Overall Framework

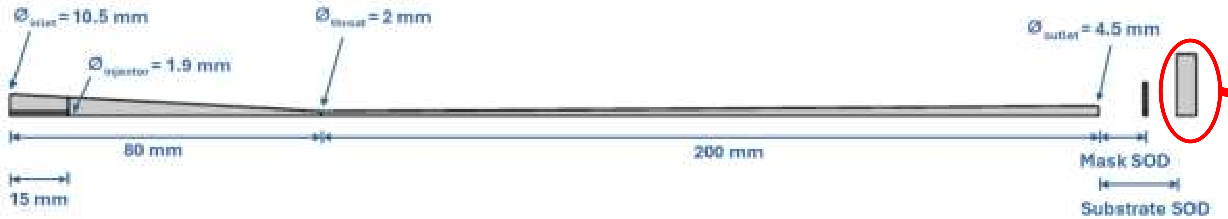


- **Why Sampling:** 48 CFD cases and $\approx 10^6$ particles on the substrate per case. Difficult to handle.

- **First-Layer Model:** KNN-KDE + physics-aware projection → <u>spatial probability distribution of particles.</u>

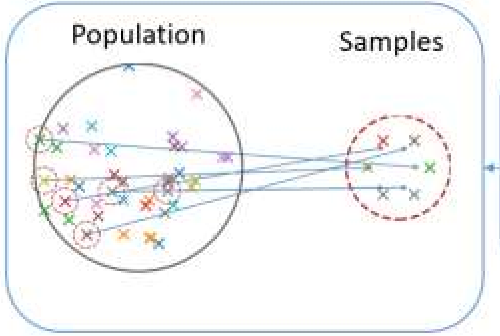
- **Second-Layer Model:** Interpolation → symbolic feature discovery → weighted random forest → <u>velocity & temperature of each particle.</u>

Sampling – Part_1



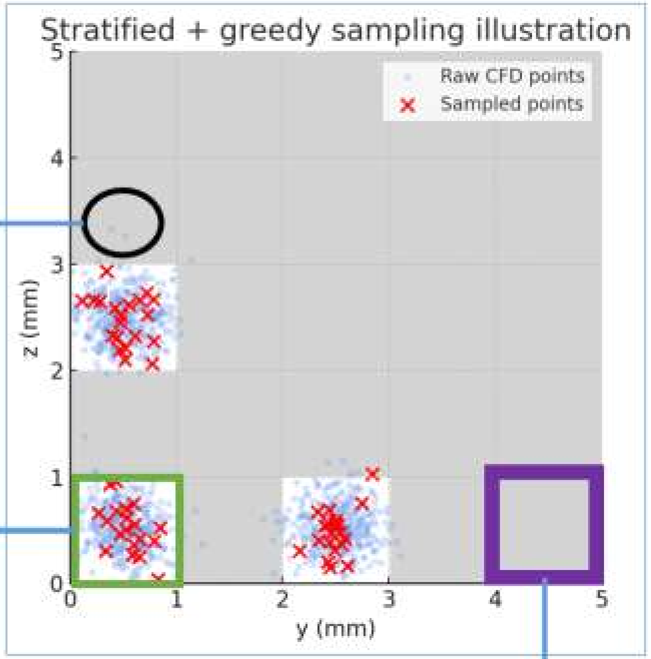
1. Multidimensional stratification bins y & z directions.

2. Greedy pick maximises diversity inside each bin.



"Particles > quota → greedy max-min selection."

"Particles ≤ quota → keep all."



"Each square represents one stratification layer."

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Sampling – Part_2

(# of stratified Layers,# of samples collected)

Genetic Algorithm searches best combination of two hyperparameters

≈5000 particles on the substrate per case

$$\text{Var Ratio}(f) = \frac{\text{Var}_{\text{sample}}(f)}{\text{Var}_{\text{orig}}(f) + \varepsilon}$$

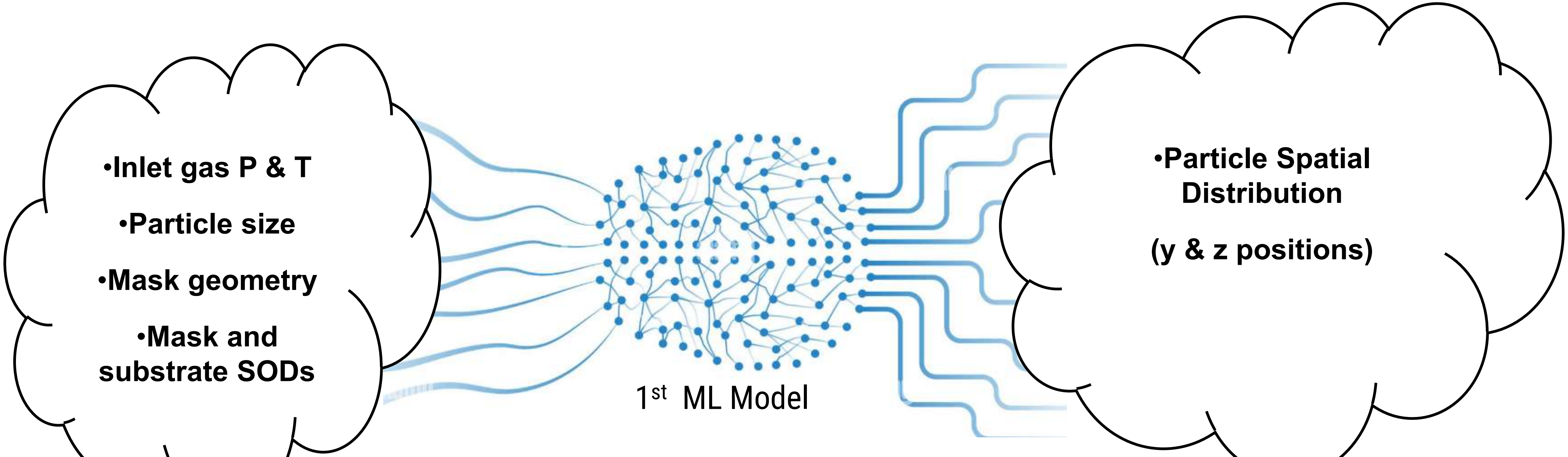
$$\text{Mean Ratio}(f) = \frac{\mu_{\text{sample}}(f)}{\mu_{\text{orig}}(f) + \varepsilon}$$

$$\text{Global Var Ratio} = \frac{1}{N}\sum_{k=1}^{N} \text{VarRatio}(f_k)$$

$$\text{Global Mean Ratio} = \frac{1}{N}\sum_{k=1}^{N} \text{MeanRatio}(f_k)$$

Quality metrics/Fitness Score

1st ML Model - Spatial Particle Distribution



The overall methodology is divided into two submodules:
Stage 1.1: a two-dimensional prediction framework that integrates local kernel density estimation (KDE) with nearest neighbor search (**Initial predictions)**
Stage 1.2: identifies unreasonable particle positions in the initial predictions and reallocating them accordingly (**Correction**)

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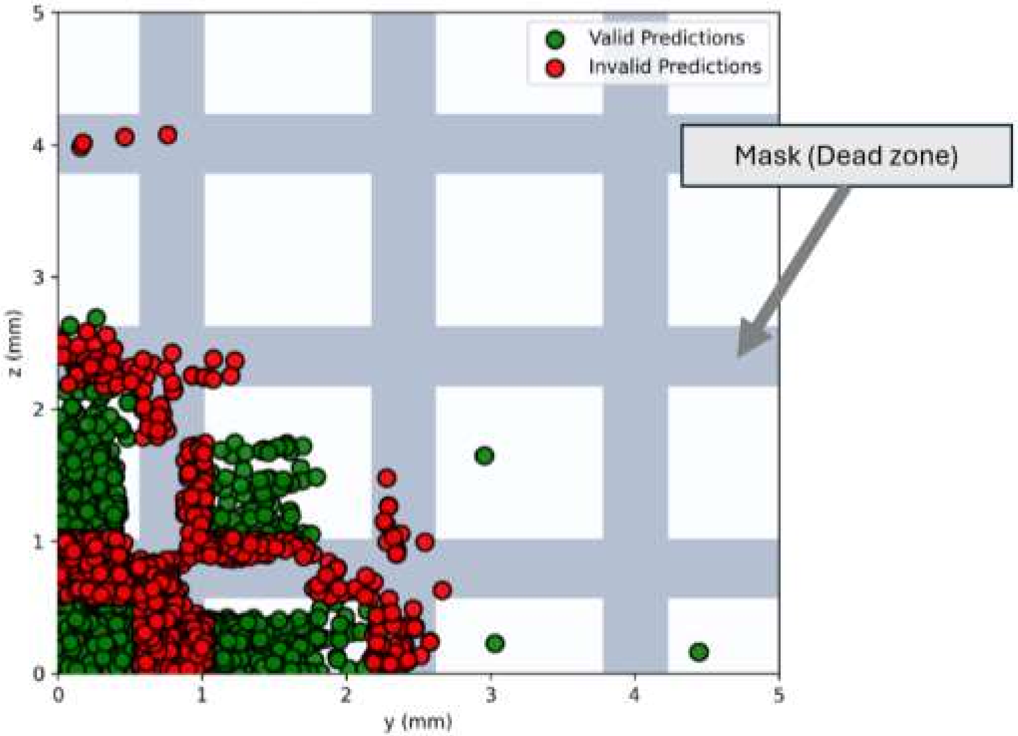
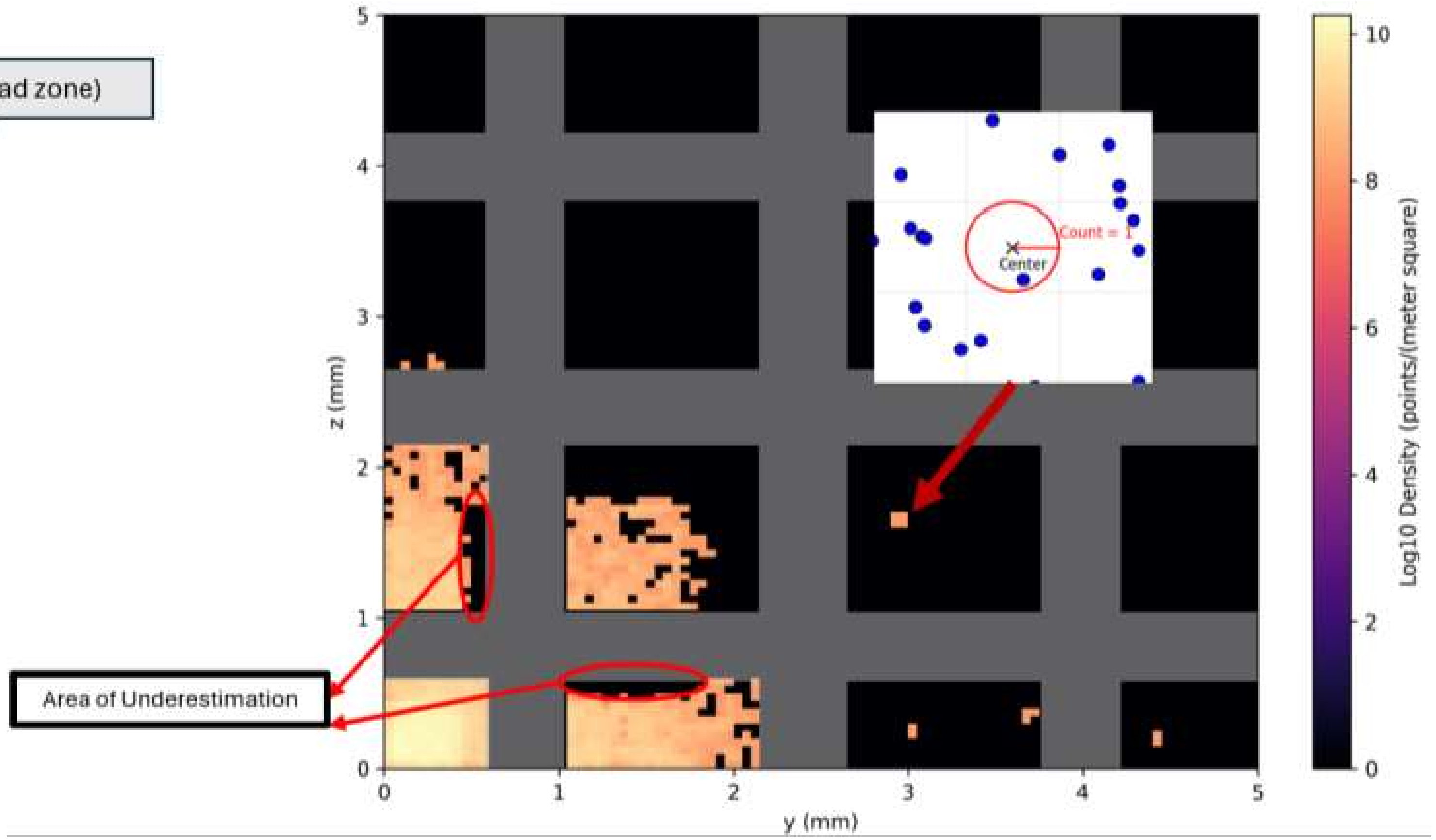
Stage 1.1: KNN-KDE based model's Prediction



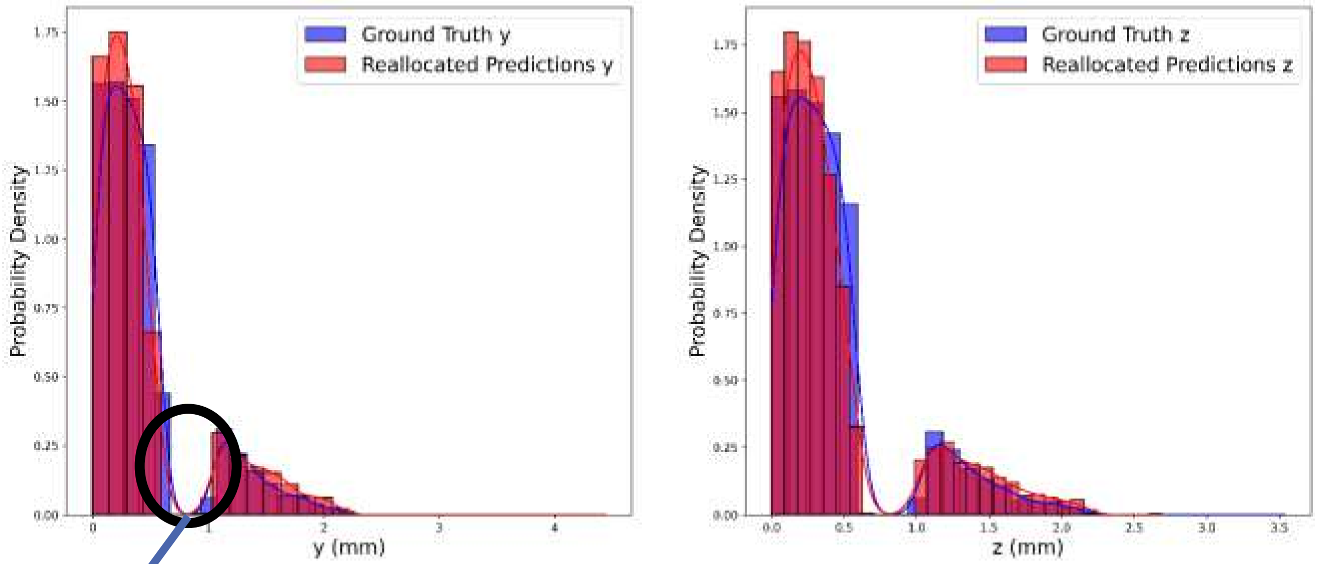


Two issues:

1. Particles located in the dead zone
2. Area of underestimation

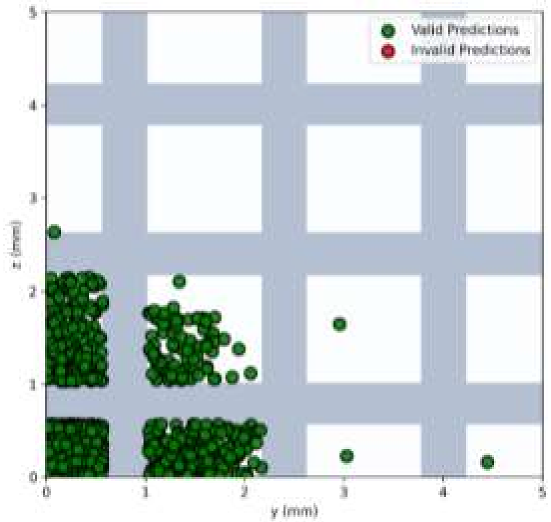
Stage 1.2: Prediction After Projection fix

(a)



FIXED !

(b)



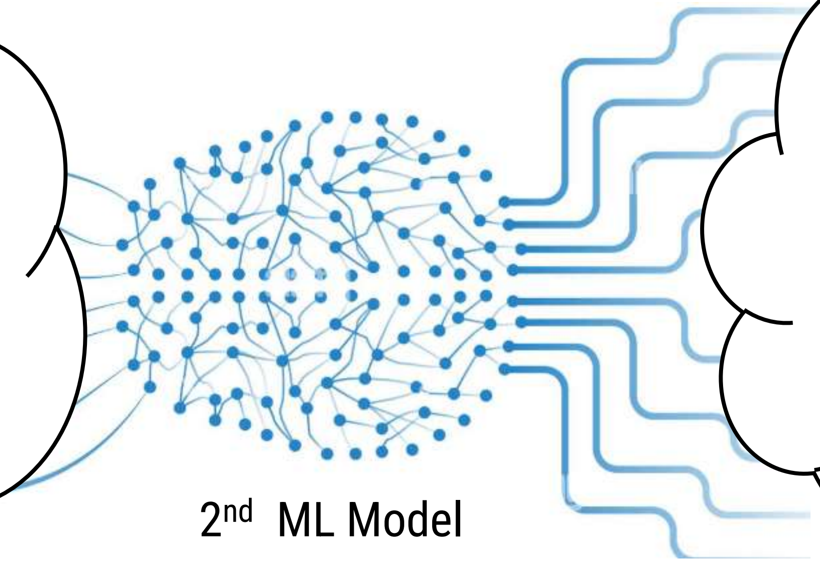
(a) Distribution of reallocated predictions vs. ground truth (y and z) for the test sample

(inlet pressure: 4 MPa, inlet temperature: 800° C, substrate SOD: 20 mm, mask SOD: 16 mm, wire diameter: 0.46 mm, opening size: 1.14 mm, open area: 51%)

(b) Local reallocation of under-estimated predictions for the mentioned test sample.

2nd ML Model - Predict V_p & T_p

- Inlet gas P & T
- Particle size distribution (PSD)
- Mask geometry
- Mask and substrate SODs
- Particle Spatial Distribution (y & z positions of particles)



- V_p & T_p Distributions

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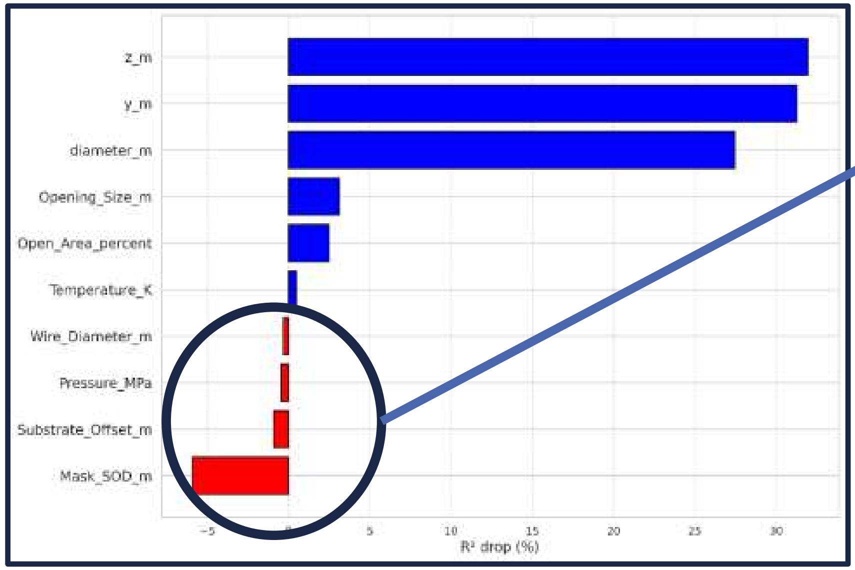
Stage 2.1 Features & Interpolation

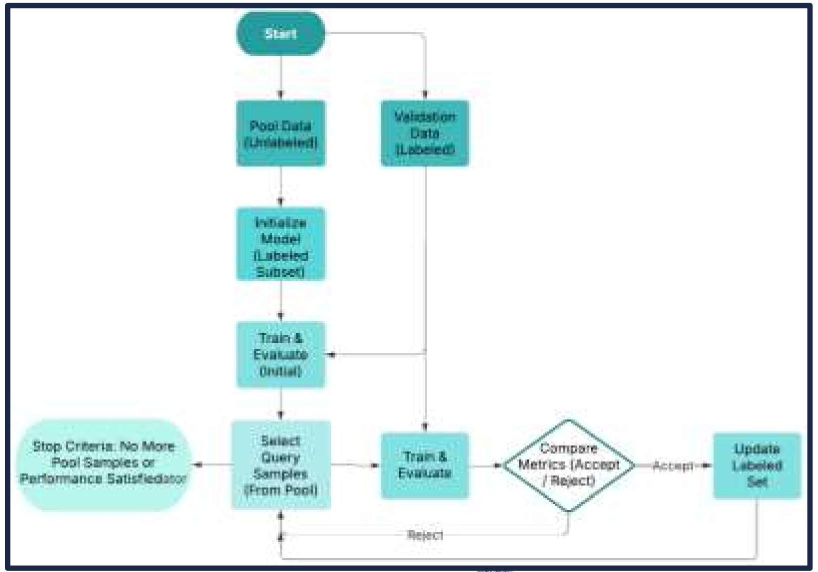


•**Issue:** Only 48 raw cases → some features show almost no variation (red bars; **contribute almost nothing to prediction**) .

•**Fix:** Interpolation generates **diverse synthetic samples**, injecting fresh variability and preventing "constant-feature" collapse in the ML model.

•**Noise control: Active-learning loop** (right) keeps only the queried samples that improve validation, yielding a clean, well-balanced training set.

- *Linear Interpolation*
- *4 Points Cubic Spline Interpolation*
- *Inverse Distance Weighted (IDW)*



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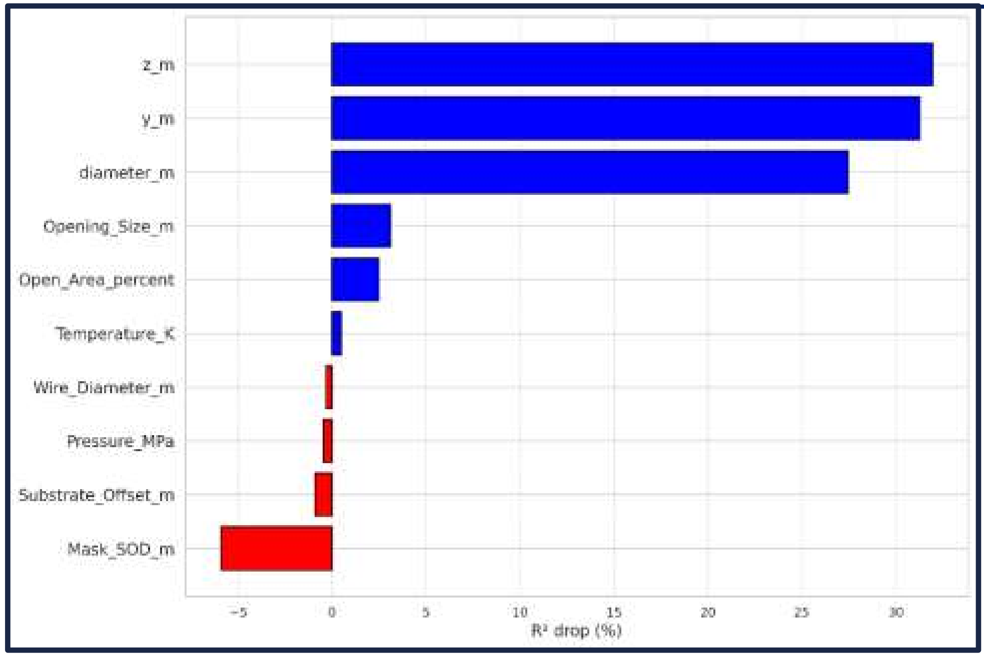
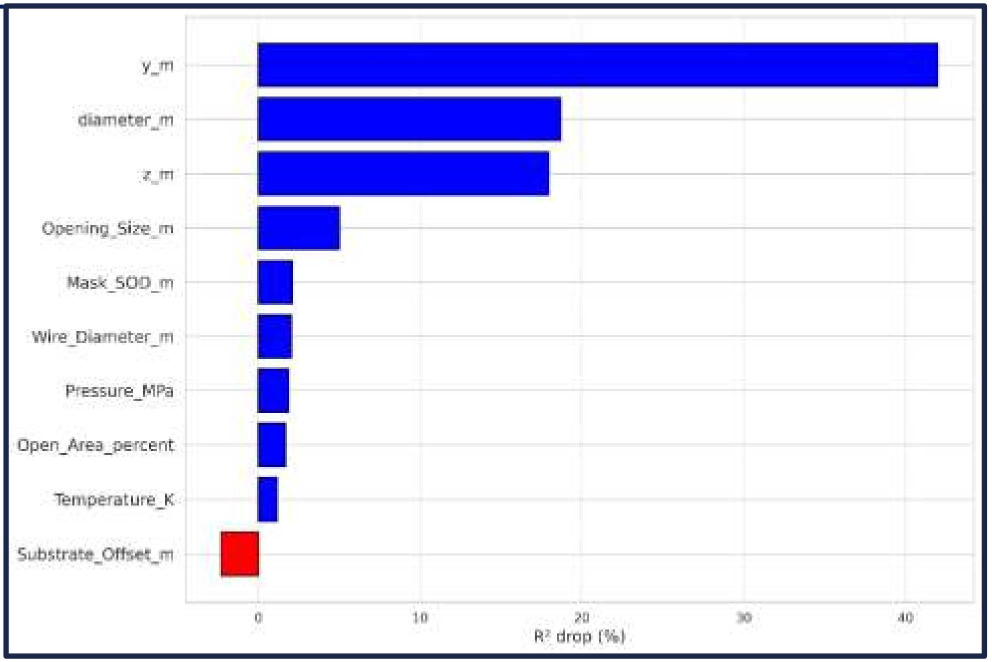
Stage 2.1 Features & Interpolation Result



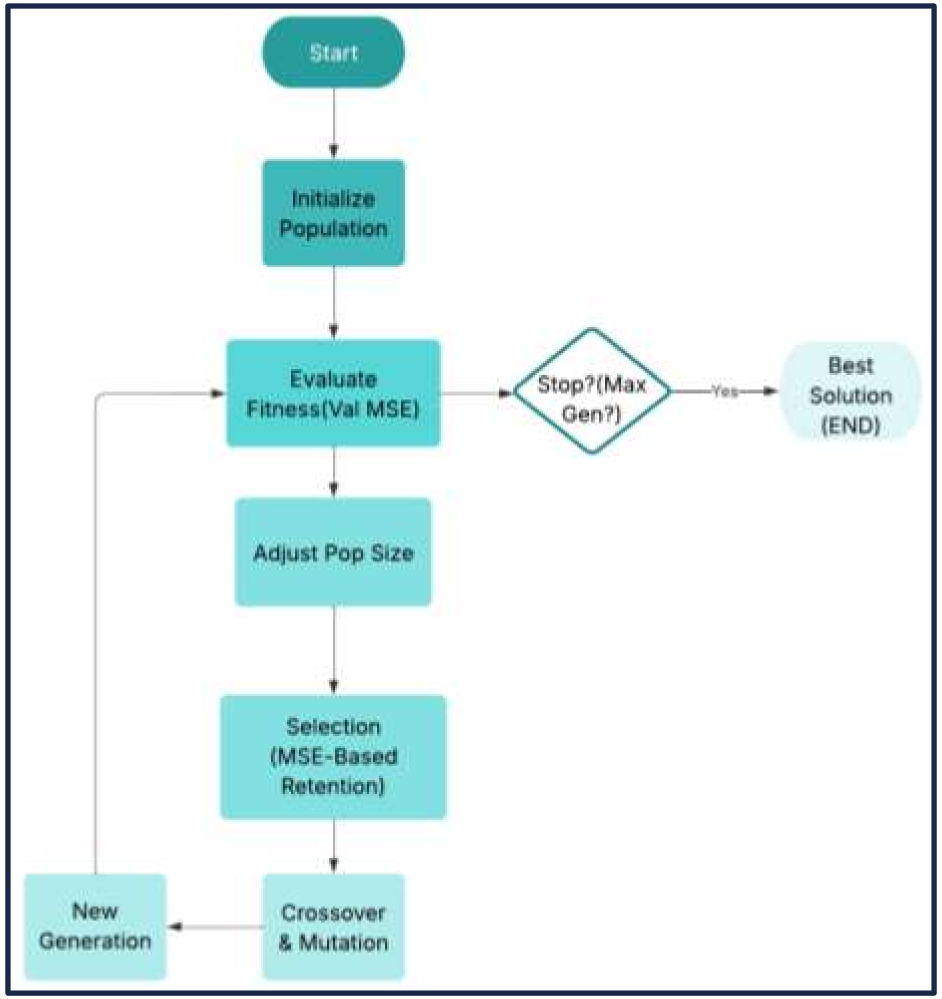


Feature importance before interpolation (left) vs. after interpolation (right).

Feature-importance changes after dataset expansion.
Right chart uses the **86 selected CFD interpolated set**; left chart show the case **without interpolated dataset**.

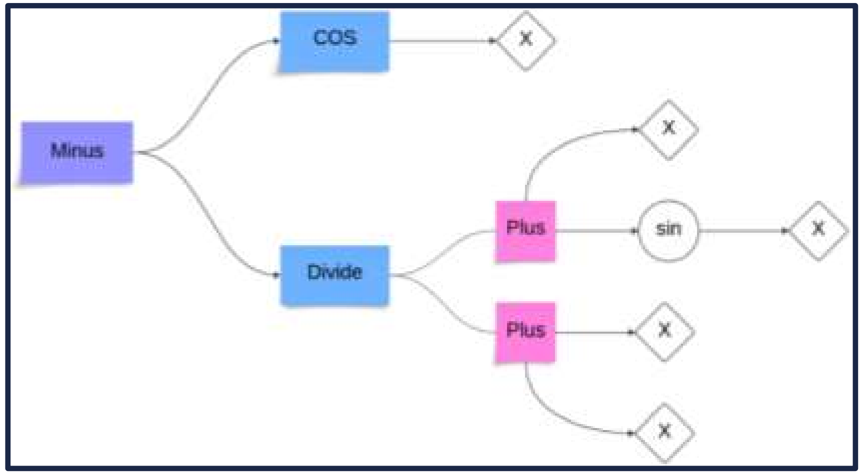
Stage 2.2 Symbolic Regression

(a)



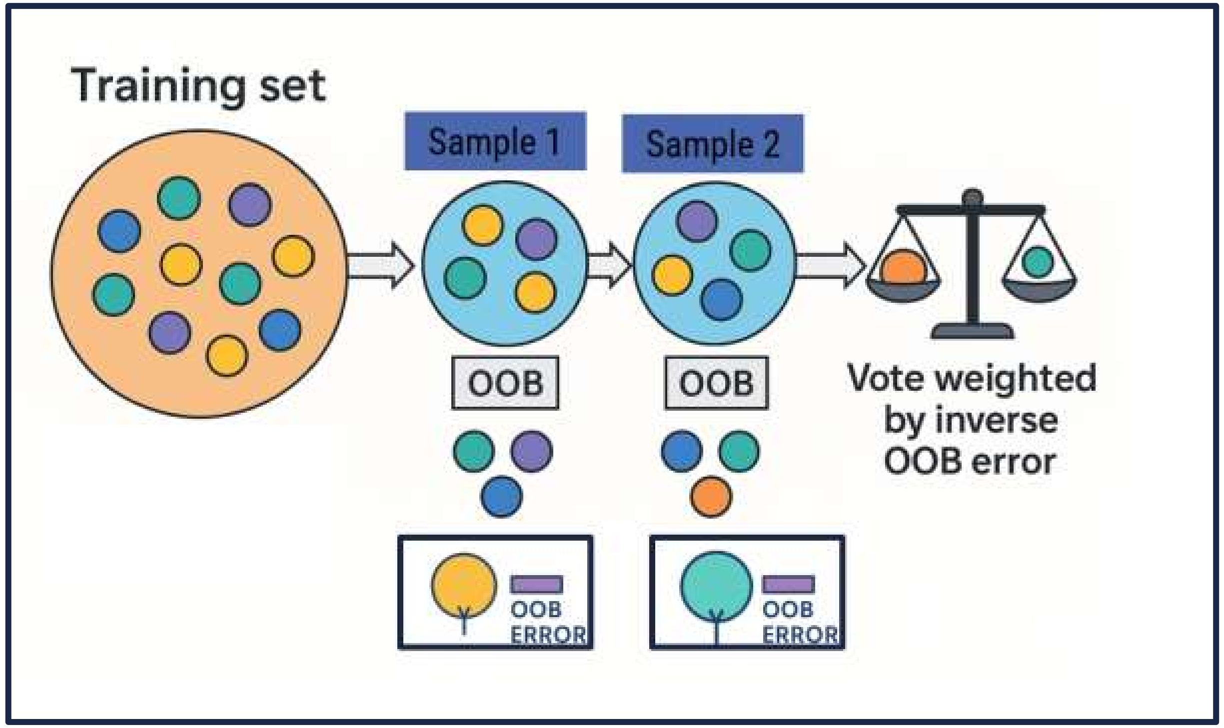
- **Genetic-programming loop** (a) evolves candidate formulas, keeps the fittest (lowest val-MSE), and breeds new ones by crossover & mutation.
- **Symbolic tree Example** (b): a compact tree mixing *cos*, *sin*, divides, and plus/minus operators to represent nonlinearities.

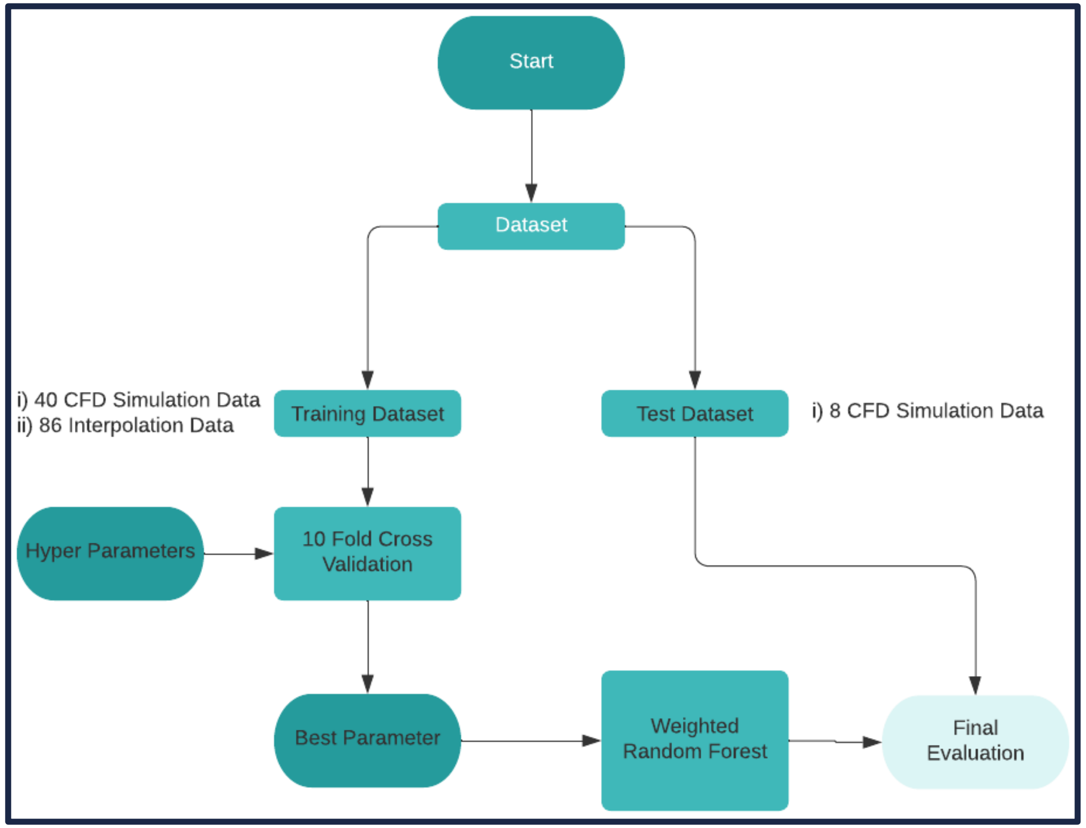
(b)



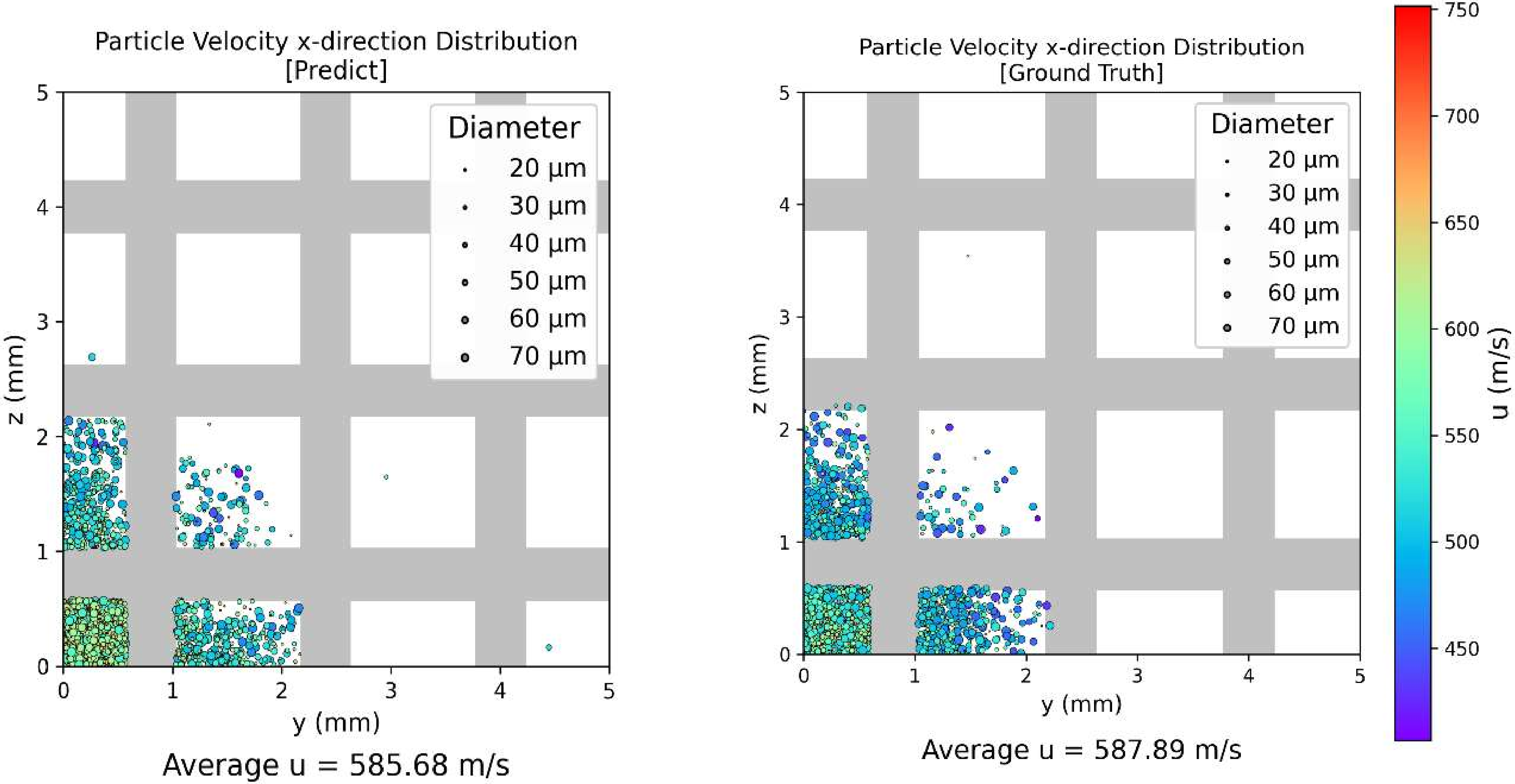
Stage 2.3 Weighted Random Forest

•**10-fold cross-validation** tunes tree depth, count, and weighting rule.
•**Weighted scheme:** each tree's vote is inversely proportional to its Out of Bag (OOB) error → down-weights weak trees, boosts robust ones.





Two-Stage ML Prediction vs. CFD Ground Truth



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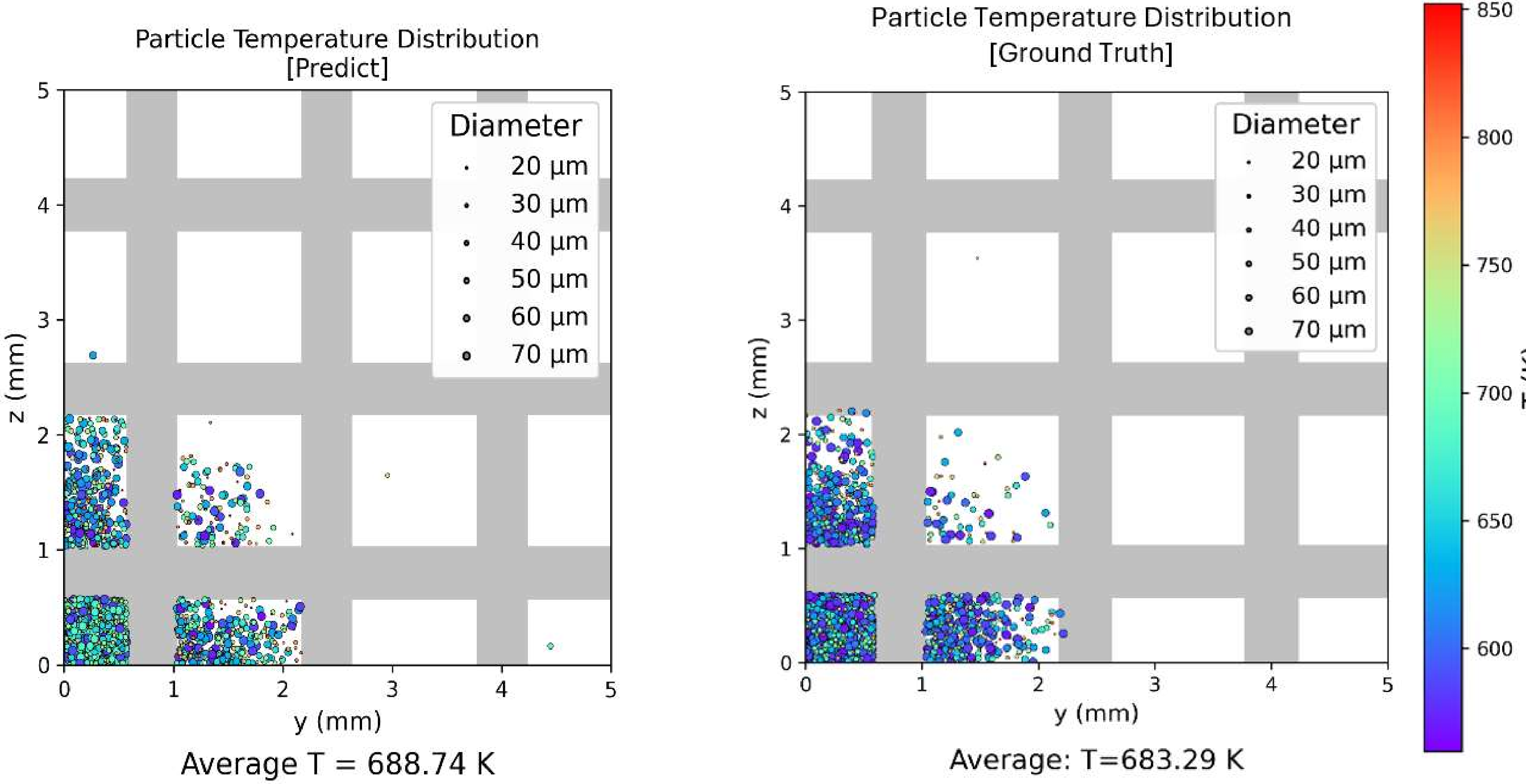
Two-Stage ML Prediction vs. CFD Ground Truth



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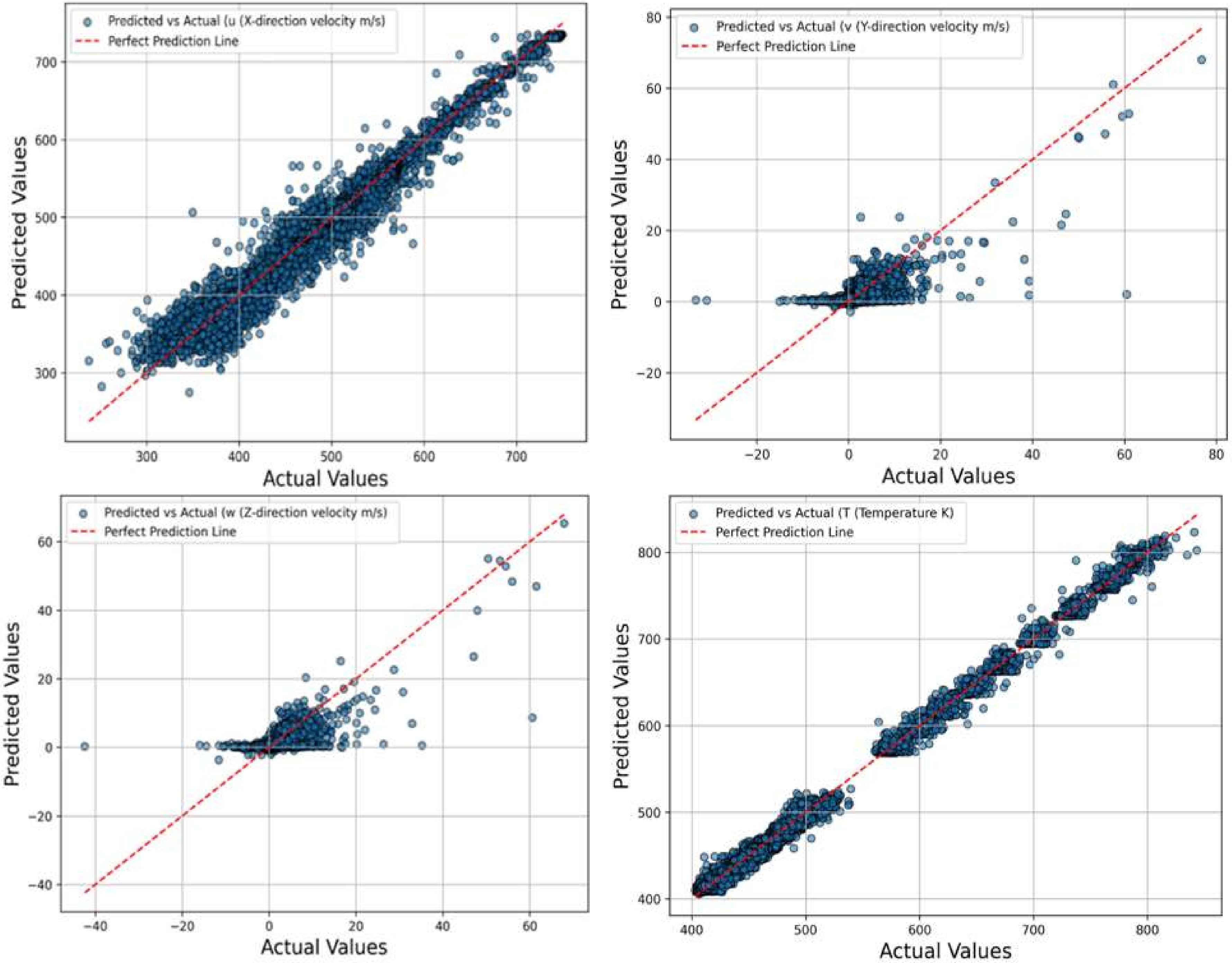
Results



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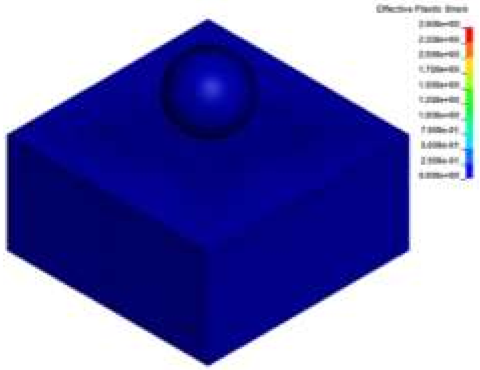
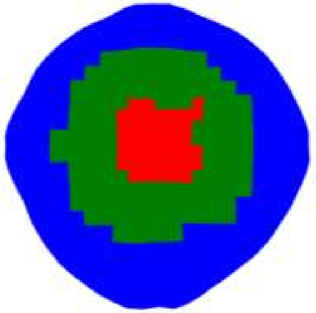
Particle impact modelling

- **Goal:** Show how ML can be used to predict the quality of a particle impacts
- Tuning spray parameters using simulation software or experimental is time consuming



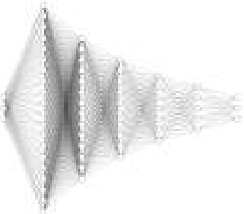
ANSYS LS DYNA

Script to Calculate Bonding using Cold Welding Criteria

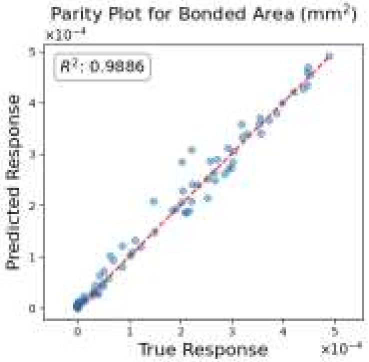


Bonding Data

- Element Status
- Bonded/De-bonded /Never bonded Areas



6-Layer Artificial Neural Network



Model to predict bonded area at any velocity and temperature

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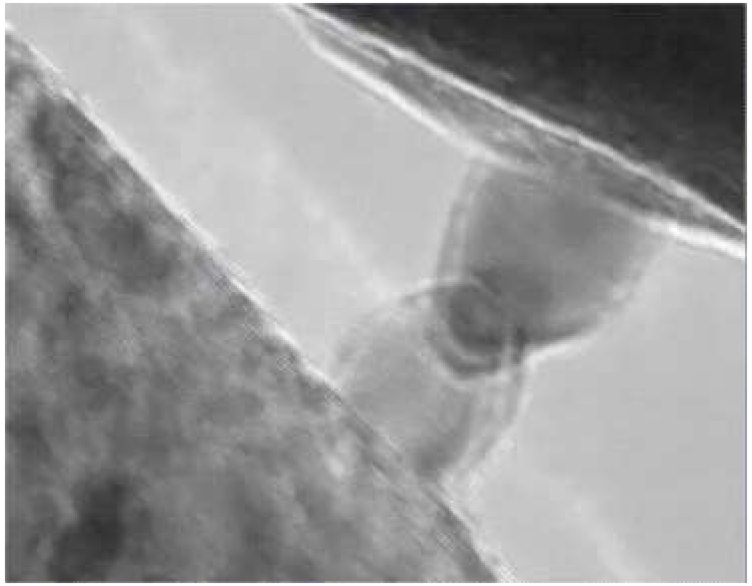
Bonding Criteria

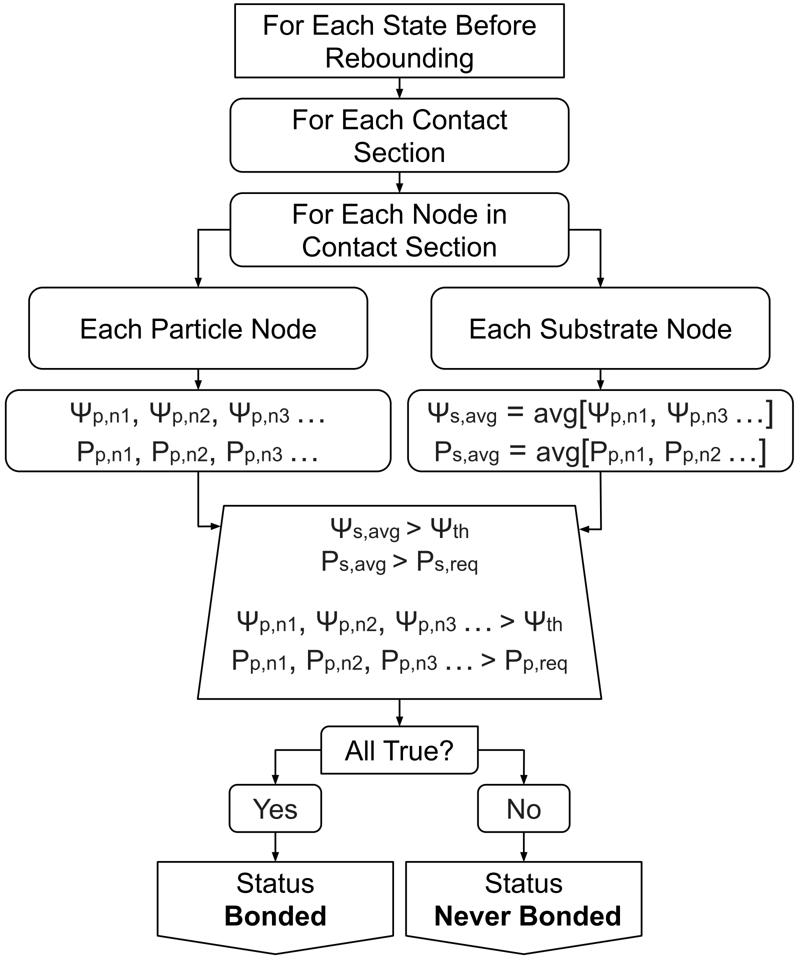
- Bonding mechanism is assumed to be similar to the one in the cold welding
- Metallurgical bonding requires intimate metal-metal contact and appropriate localized pressure
- Onset of bonding = Critical Velocity
- Ψ – Surface Expansion Factor
- P – Pressure

$$\sigma_b = P \cdot \Psi$$

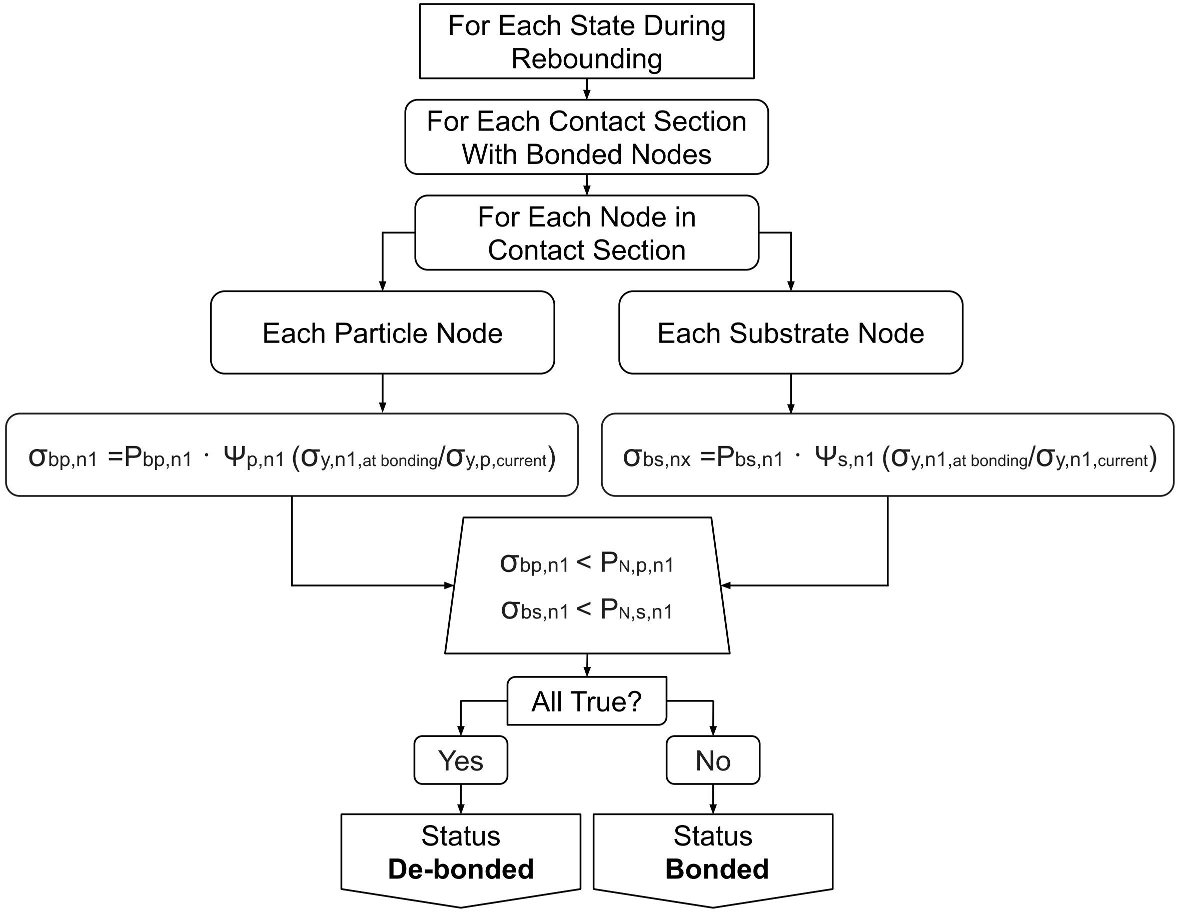


https://www.homemadetools.net/forum/cold-welding-gif-56268

Algorithm Overview



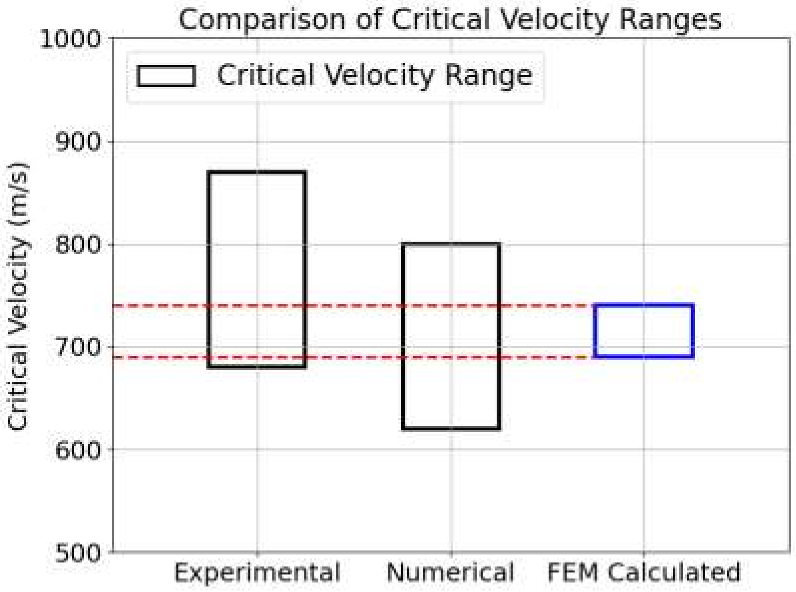
Initial Impact Phase

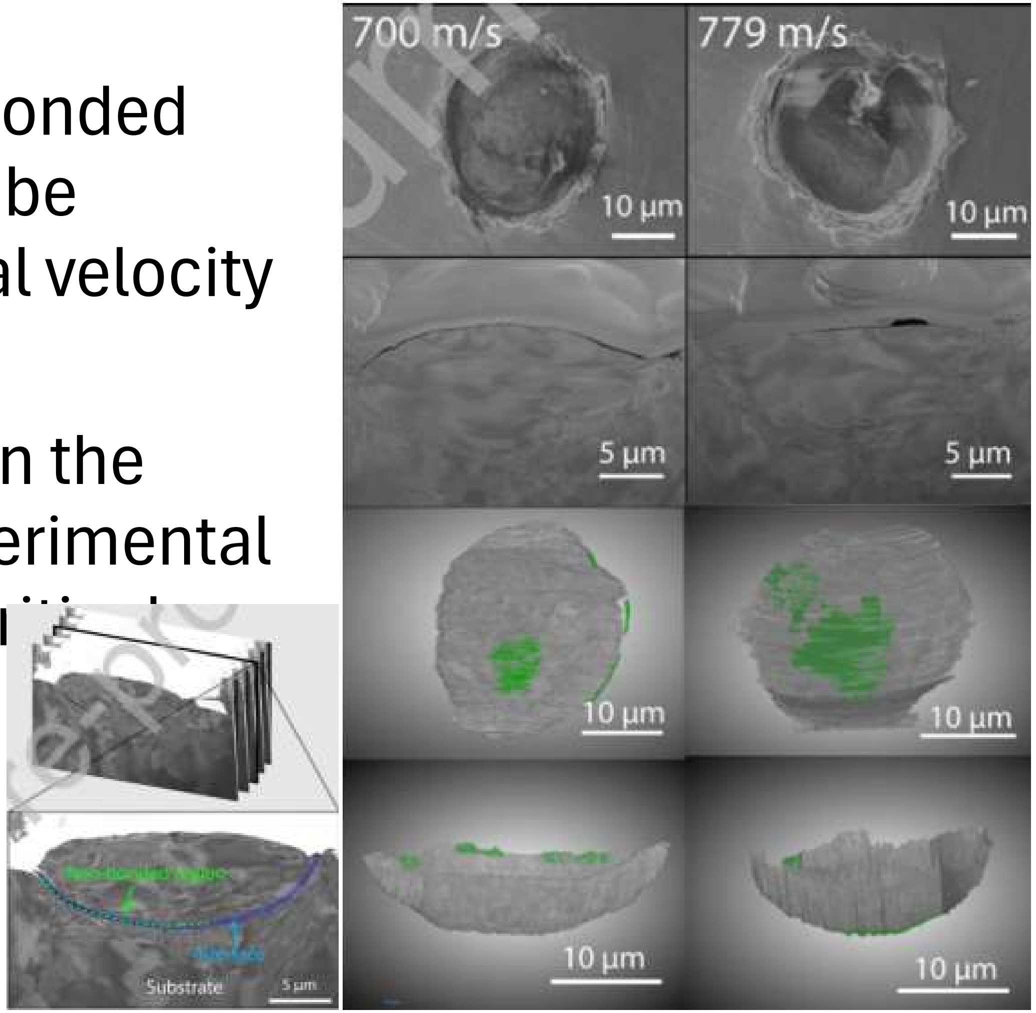


Rebounding Phase

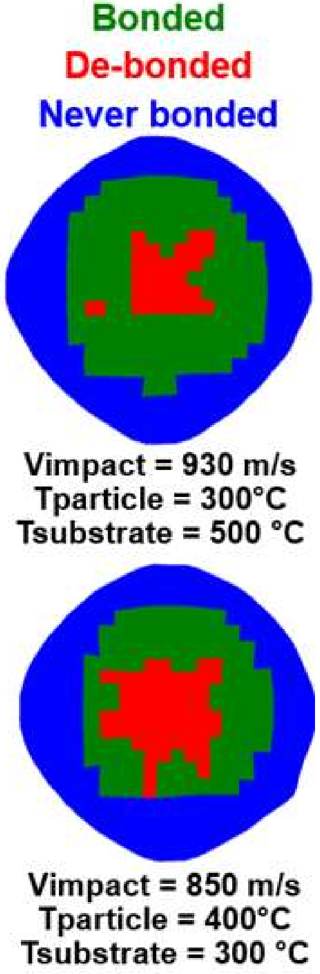
FEM Cold Welding Model Validation

- Onset of the number of bonded elements increasing can be assumed to be the critical velocity range
- Our FEM model lies within the
erimental





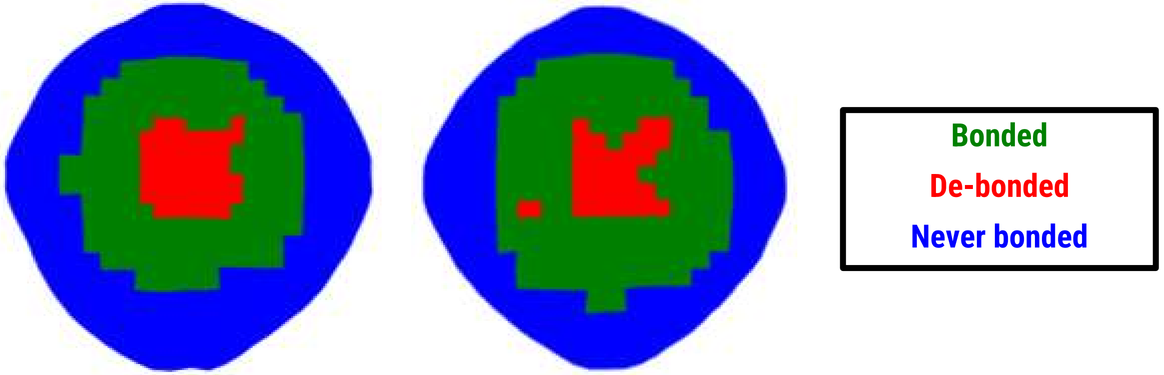
Veera Panova, Acta Materialia (2024)



Our Model

Dataset

- Varying both the substrate and particle temperat



- **Data Stored:**
  - Images of the bottom interface, element bond statuses, bonded/de-bonded areas

Particle Material	Substrate Material	Velocity Range (m/s) (+10)	Particle Temperature Range (K) (+50)	Substrate Temperature Range (K) (+50)	Total Data Points
Al-6061-T6	**Al-6061-T6**	200-1000	300-500	300-500	**1377**

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ML Model Details

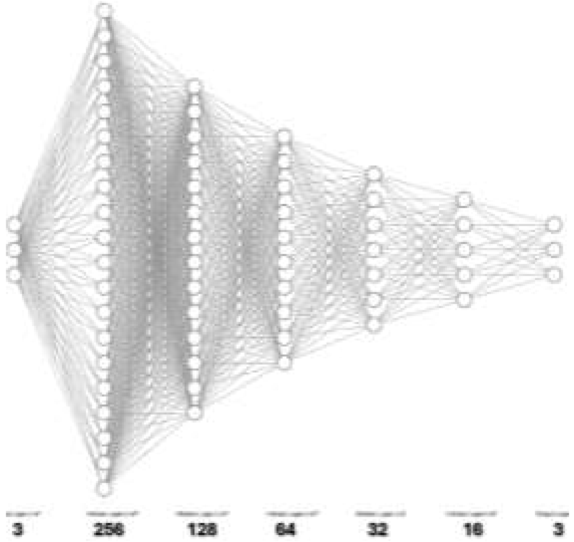
- Trained on calculated FEM bonding data
- 6-Layer Artificial Neural Network with ReLU activation function

Impact Velocity

Particle Temperature

Substrate Temperature

Inputs



Machine Learning Model

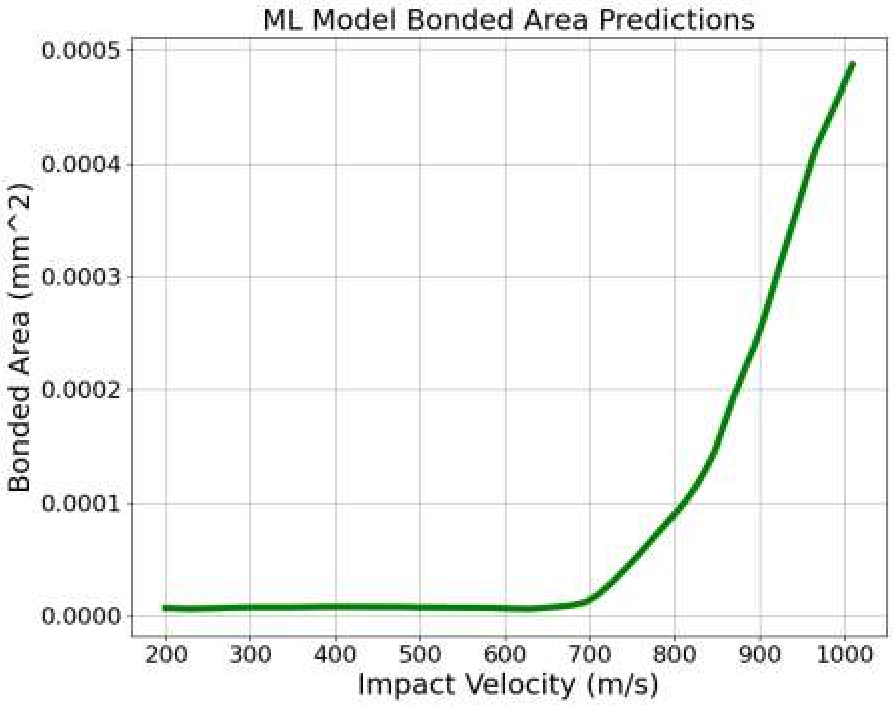
Bond Status of Interface Elements

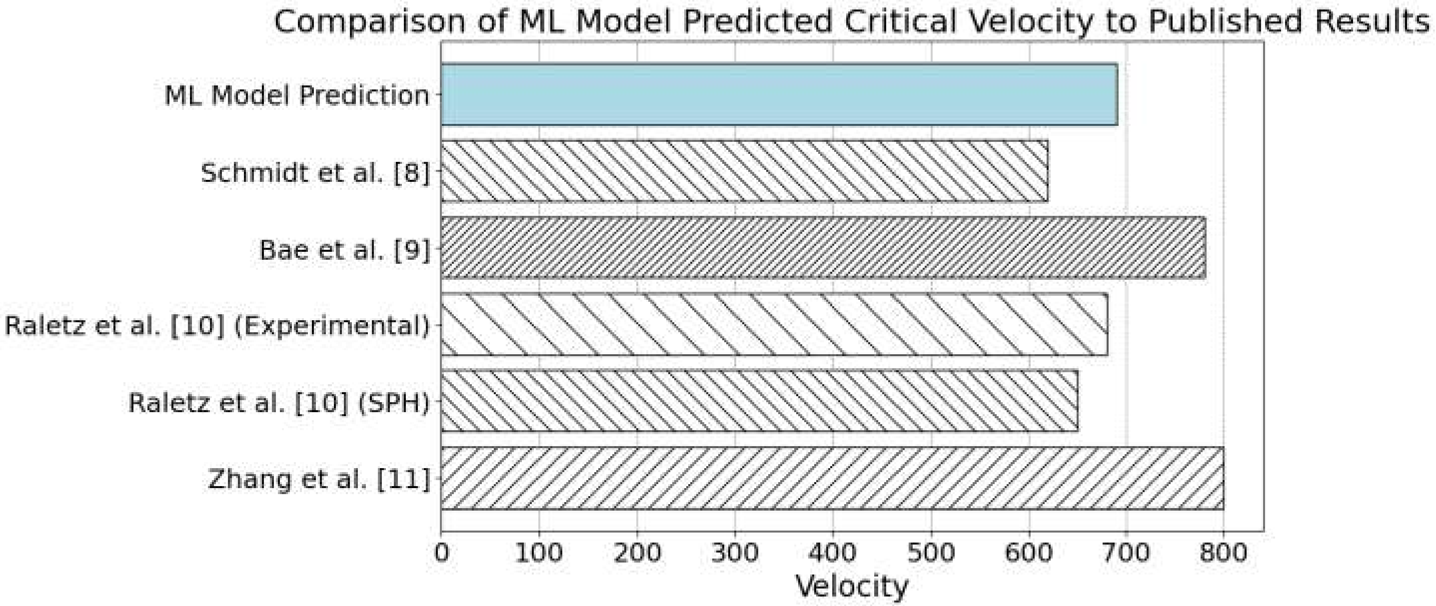
Bonded/De-bonded/Never Bonded Areas

Model Outputs

Results

- ML predicted bonded area increases drastically after 690
    - The critical velocity range for Al/Al experimentally is between 680 – 870 m/s [10]

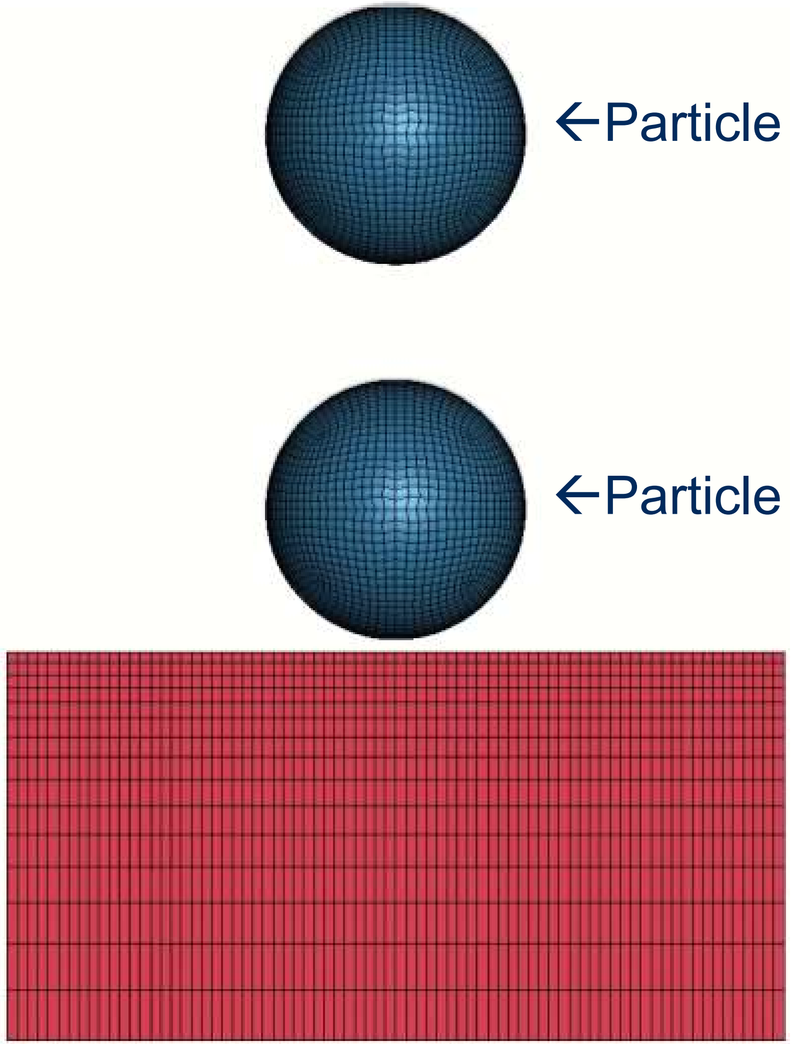


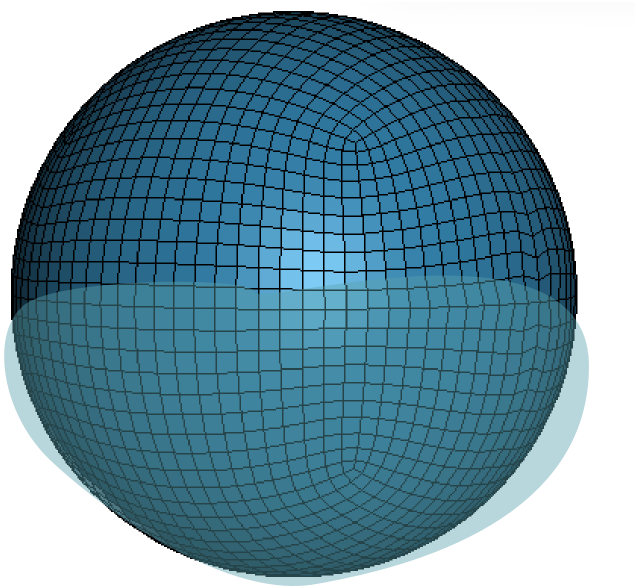


[8] Schmidt T, Assadi H, Klassen *Journal of Thermal Spray Technology (2009) 18(5-6) 794-808*
[9] Bae G, Xiong Y, Lee C *Acta Materialia (2008) 56(17) 4858-4868*
[10] Raletz F, Vardelle M, Ezo'o G *Surface and Coatings Technology (2006) 201(5) 1942-1947*
[11] Zhang J, Zhou X, Wang J *Article in Acta Metallurgica Sinica (English Letters) (2011) 24 43-53*

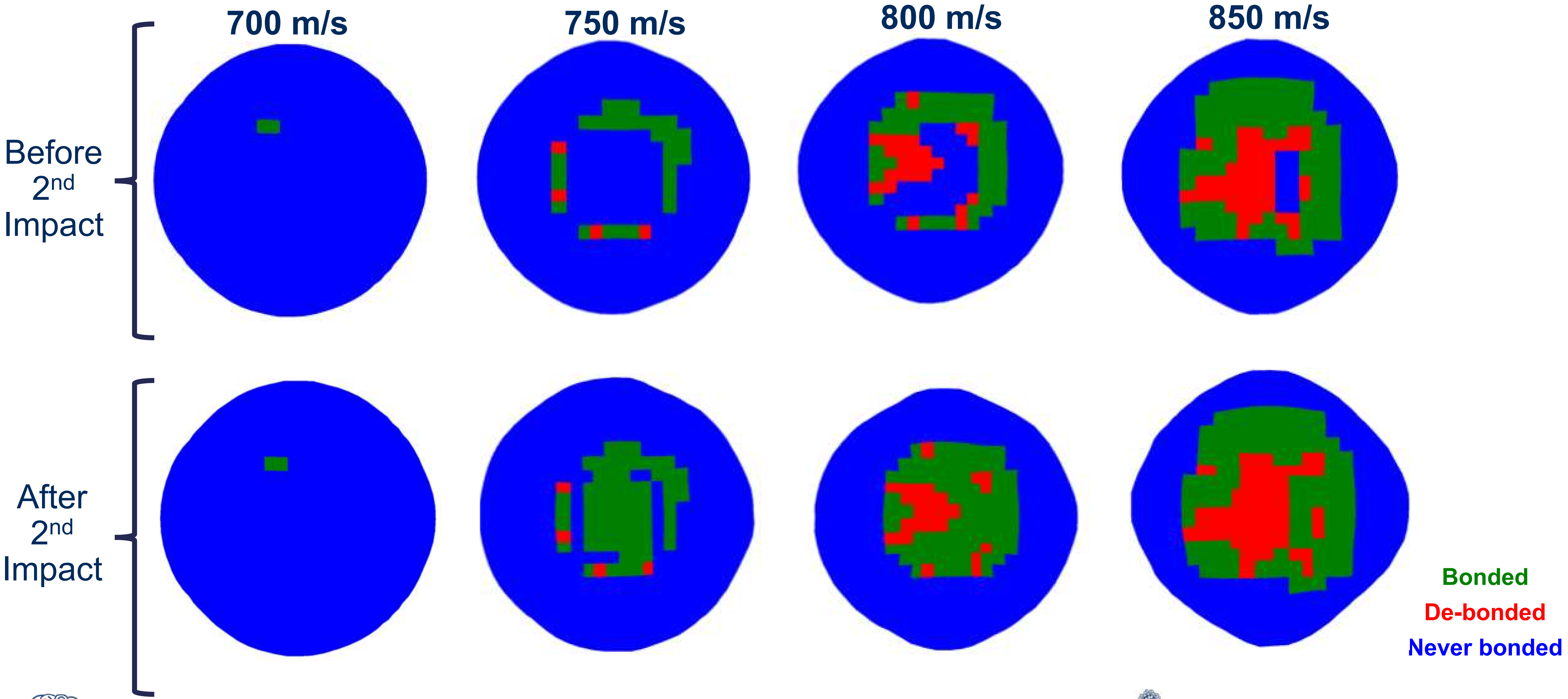
BONDING EVOLUTION FOR MULTI-PARTICLE IMPACTS

20μm Particle | 25dp | 800 m/s | Ts = 300°C





BONDING EVOLUTION



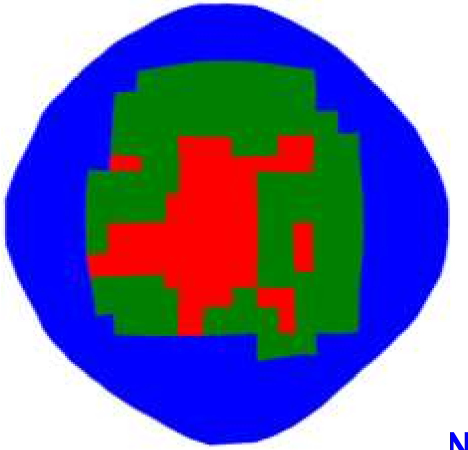
Conclusions and future work

- Reducing the runtime from ~ 18 hours using CFD to just 12 s using the above ML surrogate
  - The model attains mean absolute errors of roughly 2.2 m/s for velocity magnitude and 5.5 K for temperature

- This type of ML-based surrogate model forms a critical component of a broader digital twin (DT) framework
- With only minor parameter adjustments, the model also predicts particle distribution, impact velocity, and temperature for flat, unmasked substrates
- We anticipate that the framework can be readily extended to different powders, carrier gases, or nozzle geometries

Future Work

- Predicting bond strength of coatings using trained models on single and multi-particle impacts
- Prediction of bonded region using Generative Adversarial Networks (GAN)



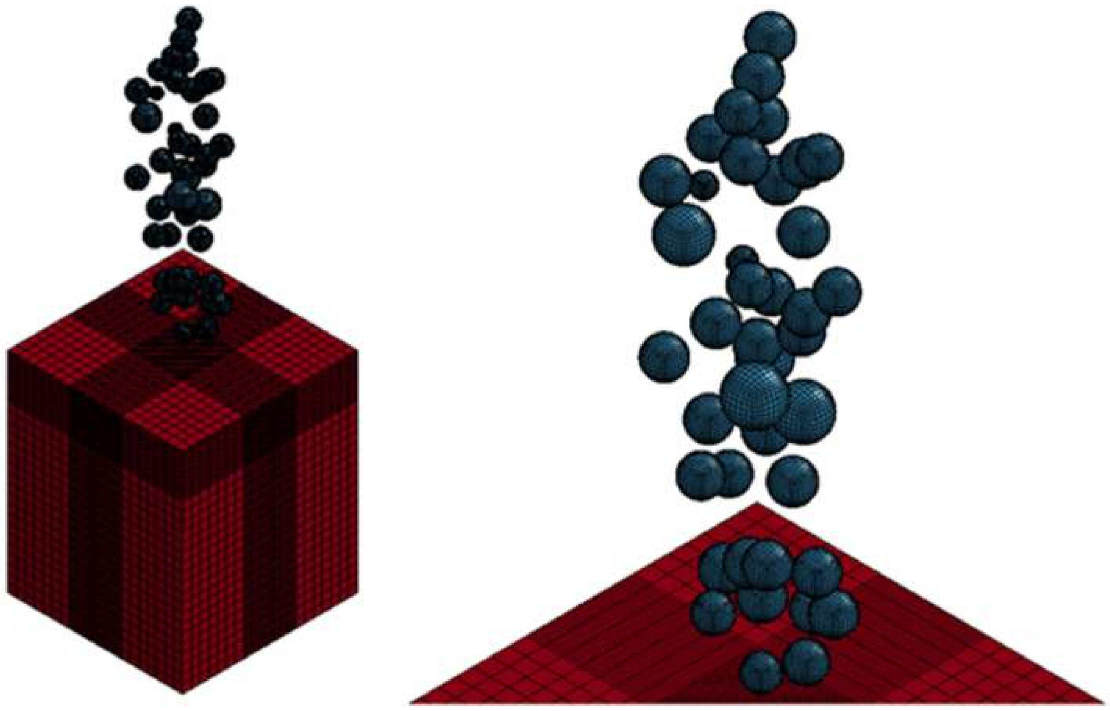


Fig. 9. Isometric view of random impact of multiple particles with different diameters.

G. Shayegan et al., Materials and Design 60 (2014)

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Thank you for your attention !

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