Using Machine Learning to Optimise the MW-PECVD Process for Polymer Substrates in Industry

Presented by Jahanzeb Khan

Thin Film Coatings

- Global market projected to reach $13.6bn by 2024
- Allows desirable properties to be applied to substrates
- Typically metal substrates are used

Diamond-like Carbon (DLC)

- Versatile - Can behave similar to diamond or graphite depending on the C-C bonds
- Desired for its hardness and Young's modulus
- Can be deposited through many different techniques

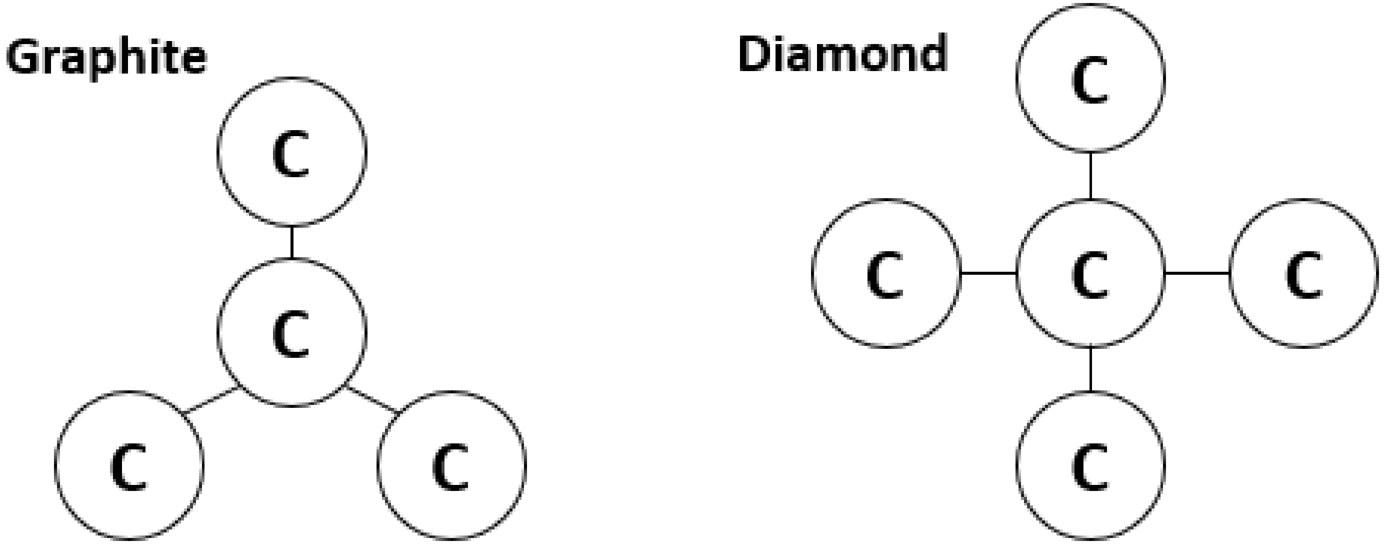

Figure 1: Structure carbon in DLC coatings

Microwave Plasma Enhanced Chemical Vapour Deposition (MW-PECVD)

- Chemical reactions between precursor (acetylene) and carrier gas (argon) take place above substrate
- Activated by plasma generated by microwave power
- Temperatures as low as 70°C
- Allows for polymer substrates to be coated

Barriers to Entry

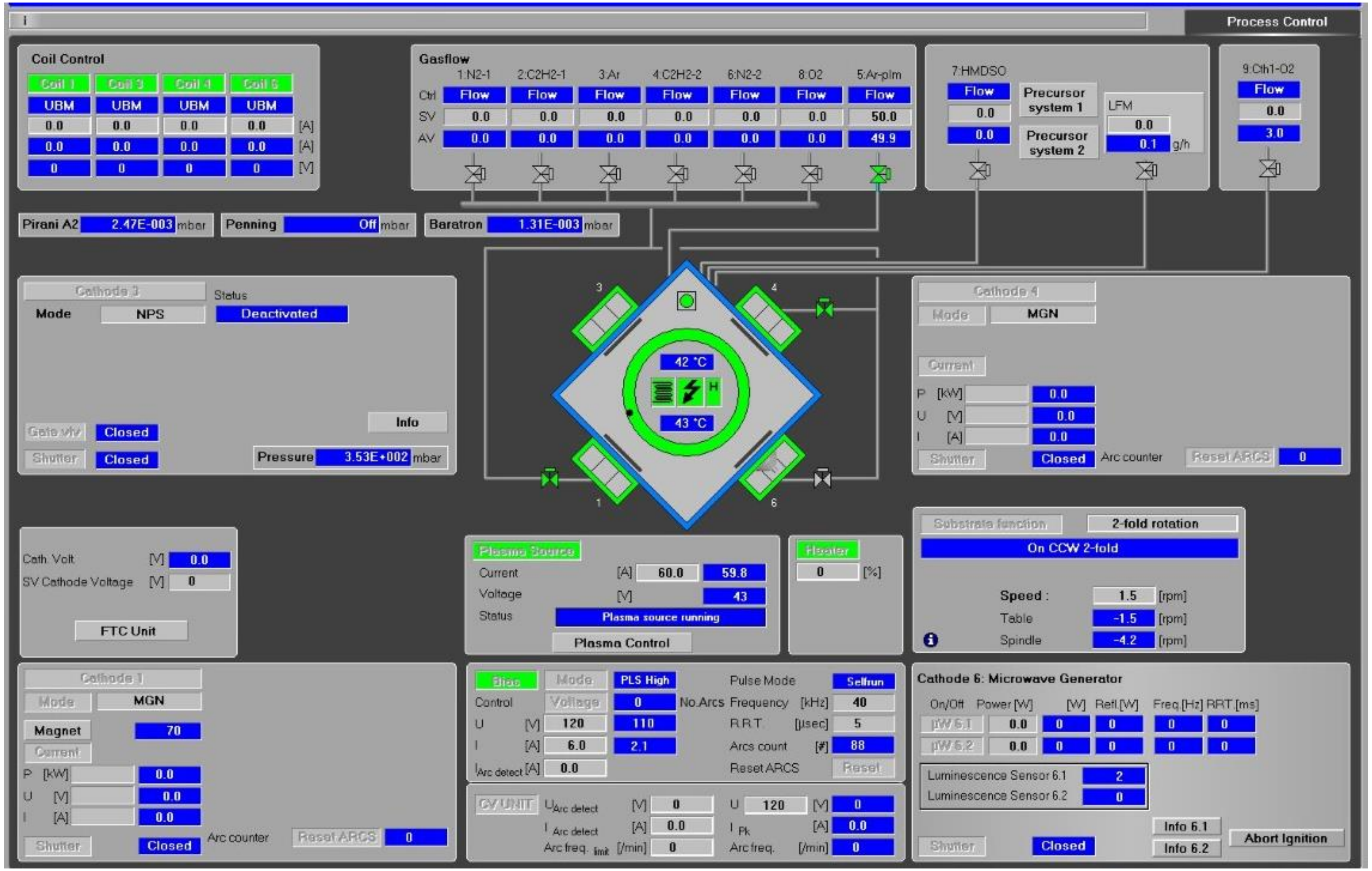

Figure 2: Hauzer Flexicoat 850 Coating System Software

Machine Learning Solutions

- Used to optimise manufacturing processes
- Reducing waste from failed attempts
- Makes tuning parameters of processes more accessible
- Use models trained on real world data to predict future outcomes
- >80% accuracy considered ‘good’

Traditional Machine Learning vs. Deep Learning

Traditional Machine Learning	Deep Learning
• Rely on simple algorithms • Coefficients are easily interpreted • Perform similar to deep learning for linear relationships	• Rely on complex algorithms • Require tuning of hyperparameters • 'Black-box' • Can identify complex relationships

Project Aims

1. Obtain real-world training data

2. Train a traditional ML model to have an accuracy of >80%

3. Train a DL model to have an accuracy of >80%

4. Compare models to assess which is more suitable

5. Develop a MW-PECVD optimisation tool

Obtaining Real-World Data

- Data obtained from study taken by Sean Michael Carley
- Limitations of Carley's methodology were recognised
- Pre-processing of data was required
- 80-20 training/testing data split

MW Power (W)	Working Pressure (mbar)	Gas Flowrate Ratio (%C2H2)	Hardness (GPa)	Young's Modulus (GPa)
1032	0.012	94	4.9	21.9
1087	0.011	92	4.1	19.8
1032	0.011	85	3.4	19.2
1087	0.009	40	2.1	14.0

Figure 3: Training Dataset Extract

Multi-Linear Regression (MLR) Model

- Ordinary Least Squares (OLS) Regression
- Coefficients were extracted and compared to literature

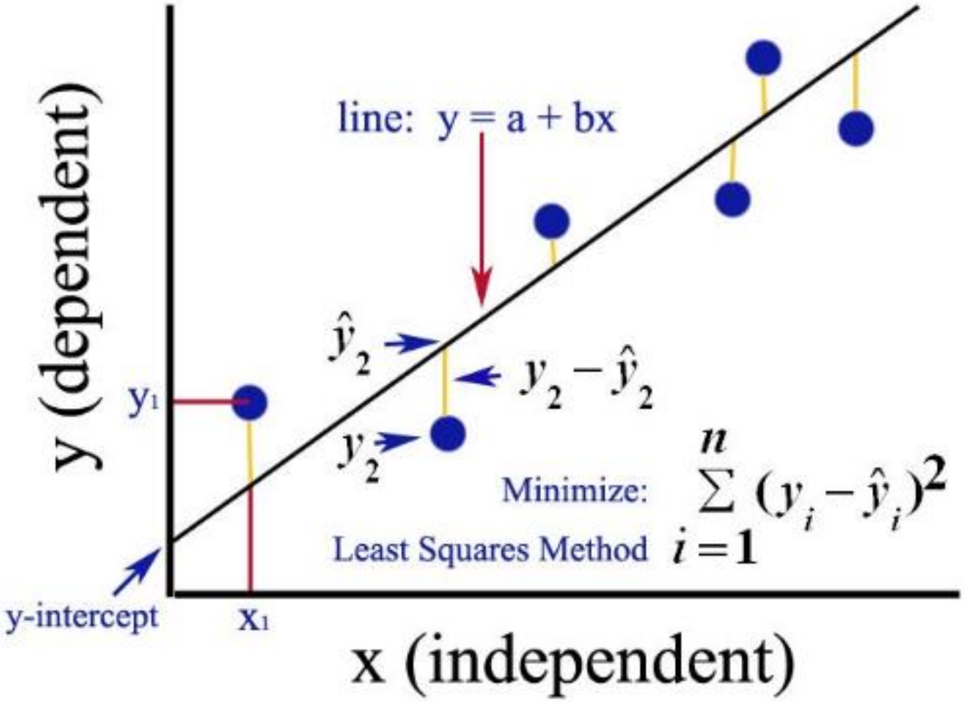

Figure 4: Ordinary Least Squares Regression Method

Training MLR Model

Deposition Parameter	**Coefficient for Hardness**	**Coefficient for Young's Modulus**
MW Power	0.27	1.33
Working Pressure	1.14	4.41
Gas Flowrate Ratio (%C2H2)	1.73	4.86

Testing MLR Model

Hardness (GPa)		Young's Modulus (GPa)	
Actual	**Predicted**	**Actual**	**Predicted**
2.5	3.0	13.5	18.5
4.1	4.1	24.8	21.1

Mean Average Percentage Error (MAPE) = 18%

Accuracy = 82%

Multi-Layer Perceptron (MLP) Model

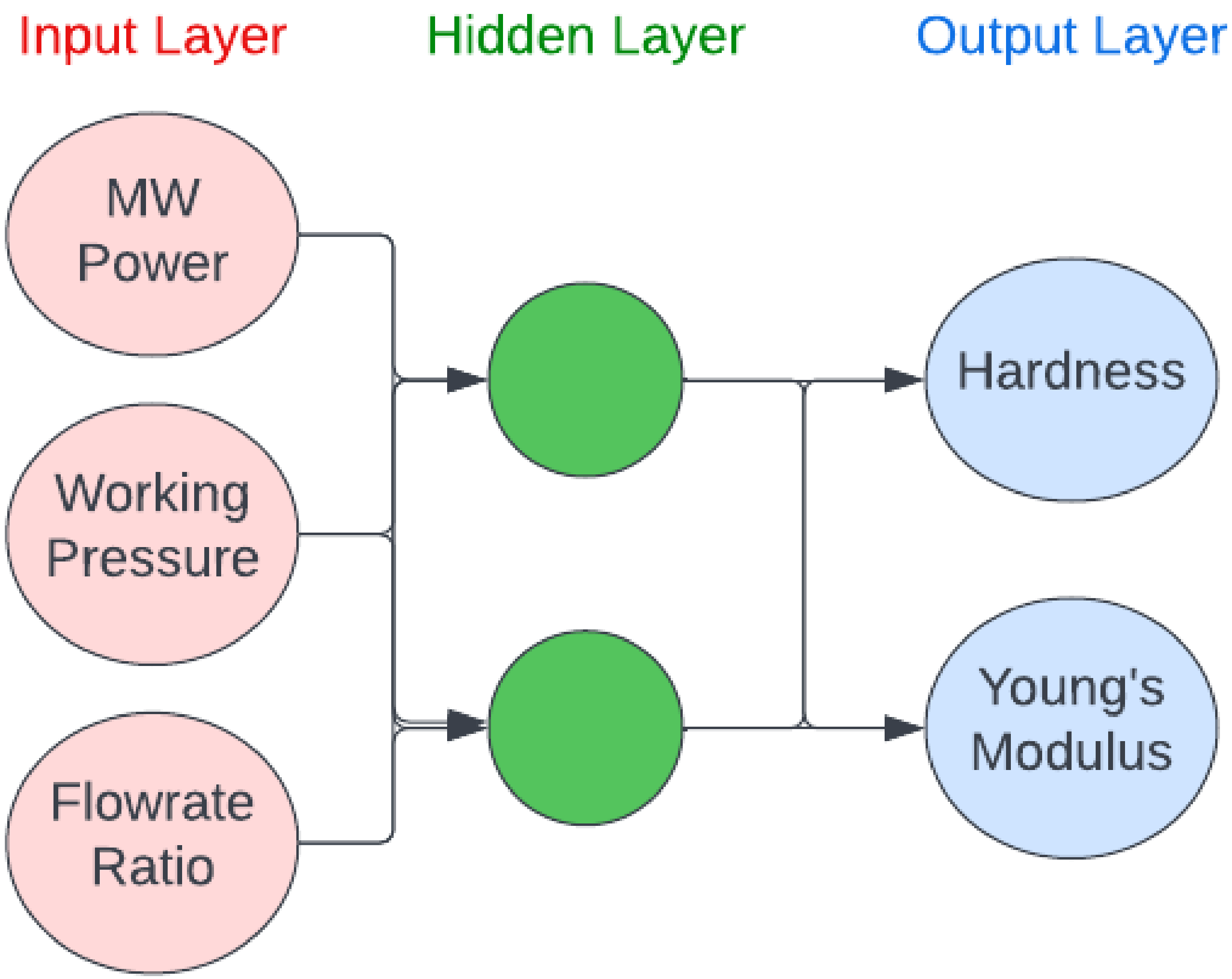

Figure 5: Deep Learning Model Diagram

Training MLP Model

Tuning hyperparameters:

- No. of Neurons
- No. of Hidden Layers
- Activation function
- Solver method
- Convergence conditions
- Random state

Training MLP Model

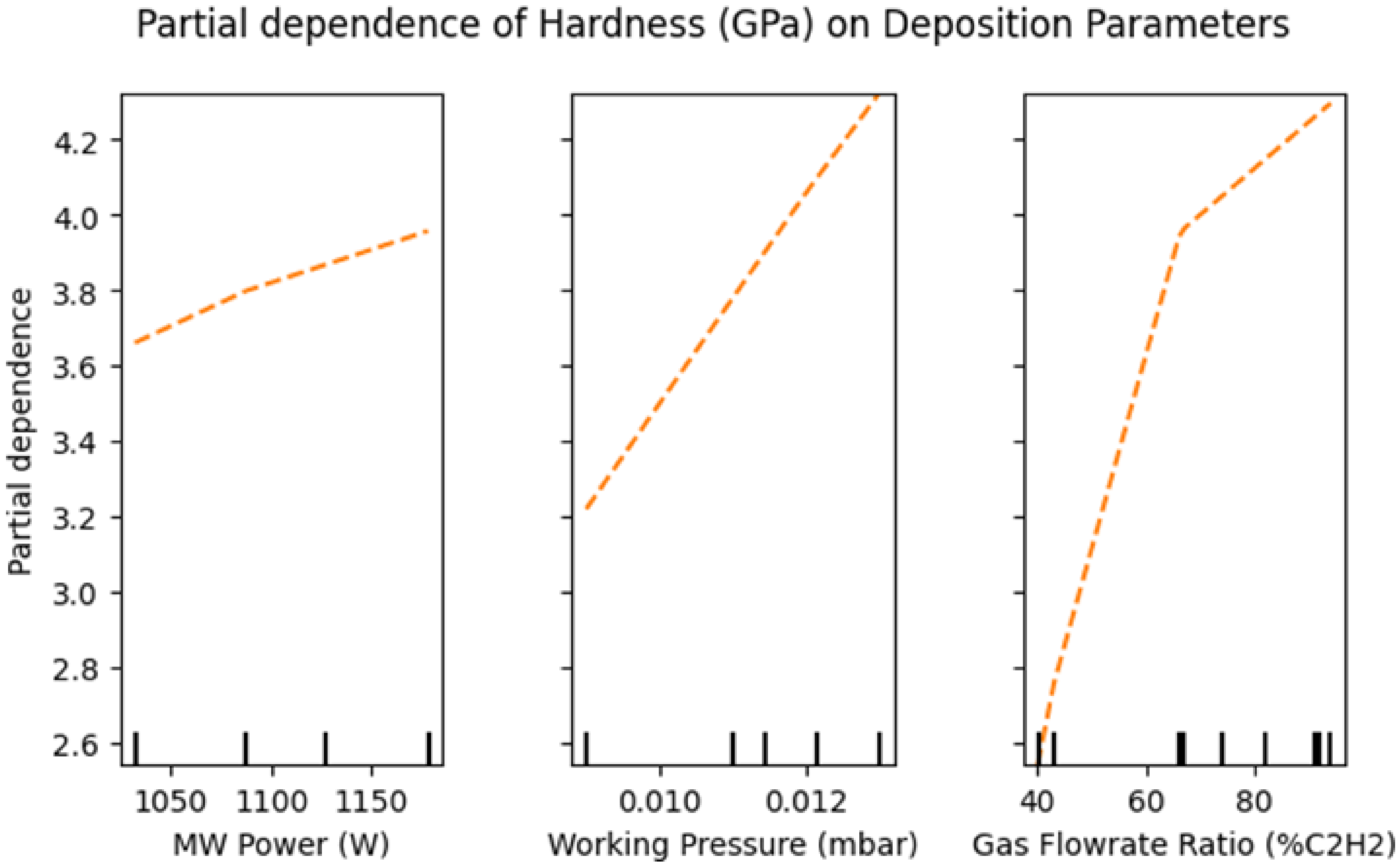

Figure 6: Partial Dependence Plots of Hardness

Training MLP Model

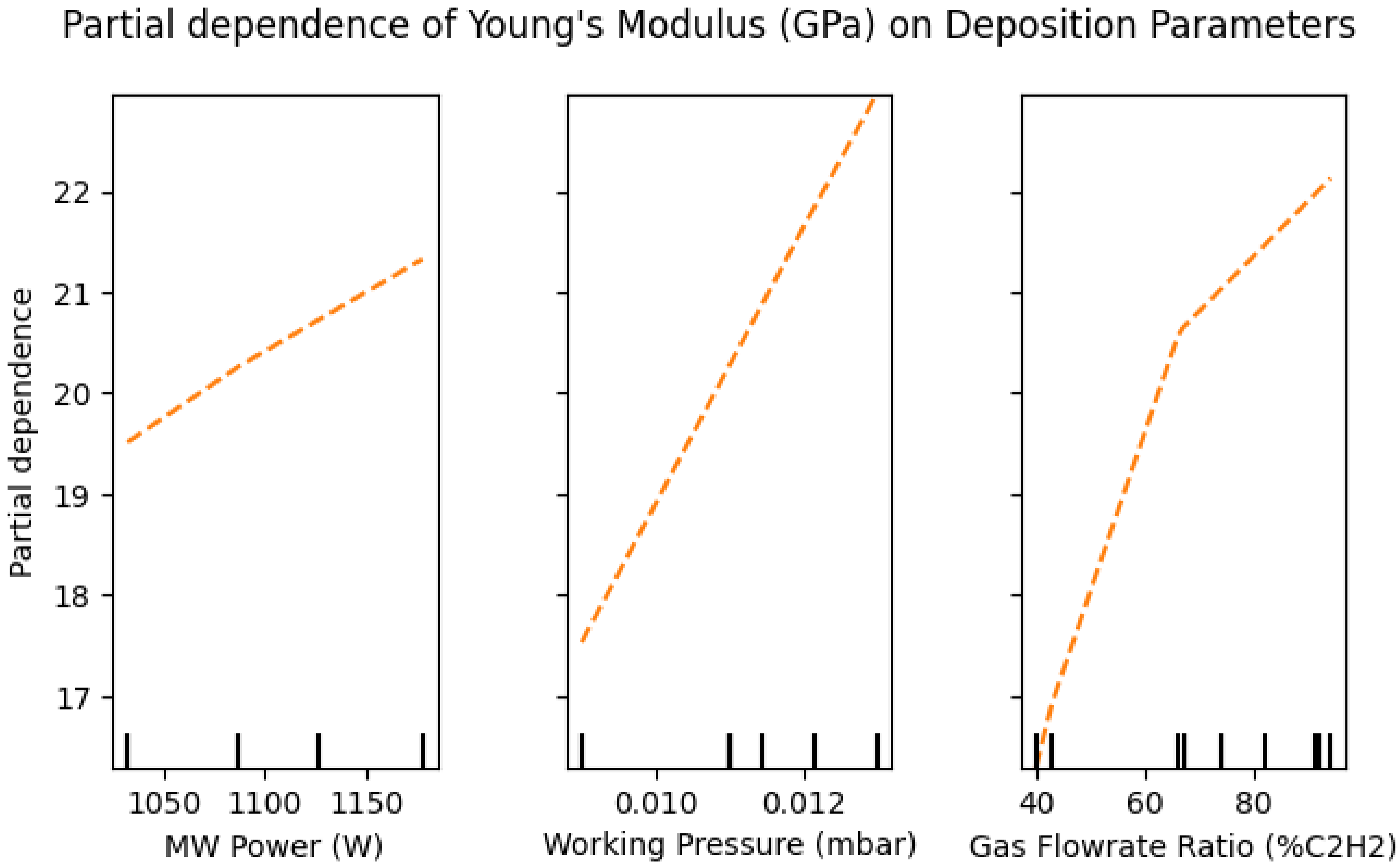

Figure 7: Partial Dependence Plots of Young’s Modulus

Testing MLP Model

Hardness (GPa)		Young's Modulus (GPa)	
Actual	**Predicted**	**Actual**	**Predicted**
2.5	2.5	13.5	16.9
4.1	3.9	24.8	20.6

Mean Average Percentage Error (MAPE) = 12%

Accuracy = 88%

Comparison of Models

Traditional Machine Learning	Deep Learning
• 82% accuracy • Coefficients can be explained by literature • 0.0056s to train	• 88% accuracy • PDP plots closer match literature • Most PDP plots show non-linear • 0.57s to train

Developing Optimisation Tool – Program A

1. Train MLP model
2. Generate lookup table of all possible MW-PECVD parameter combinations within range of training data
3. Add predicted properties to parameters in lookup table
4. Output lookup table to csv

MW Power (W)	Working Pressure (mbar)	Gas Flowrate Ratio (%C2H2)	Hardness (GPa)	Young's Modulus (GPa)
1033	0.009	89	4	21.6
1033	0.009	90	4	21.7
1033	0.009	91	4	21.8
1033	0.009	92	4.1	21.9
1033	0.009	93	4.1	22.1
1033	0.009	94	4.2	22.2
1033	0.01	40	2.2	15

Figure 8: Lookup Table Extract

Developing Optimisation Tool – Program B

1. Take user input for desired hardness and Young’s modulus and ensure it’s within boundaries of lookup table
2. Iterate through lookup table to find parameters which minimise power usage, pressure and acetylene percentage
3. Output parameters to user along with limitations of model used

Developing Optimisation Tool – Program B

```
Enter desired Hardness of DLC coating in GPa between 2.1GPa and 5.1GPa:10
Hardness value entered is above range of this tool
Enter desired Hardness of DLC coating in GPa between 2.1GPa and 5.1GPa:4
Enter desired Young's Modulus of DLC coating in GPa between 15.0GPa and 25.3GPa:20.5

Most economic settings to achieve a Hardness of 4.0GPa and a Young's Modulus of 21.5GPa
Power (W): 1032.0
Working Pressure (mbar): 0.009
Gas Flowrate Ratio (%C2H2): 89.0

These predictions are made based on data obtained using a Hauzer Flexicoat 850 Coating
system with no bias applied across the substrates used and no measurements taken of the
self-bias applied
```

Figure 9: Program B User Interface

Concluding Comments

- Trained the models to be >80% accurate
- Determined DL to be better suited
- Used the DL model to develop an optimisation tool
- Further work: Certain deposition parameters not considered in model and flowrate values given as ratio

Thank you