Application of machine learning for predicting gas adsorption on a solid surface: Implication for CCUS projects in coal formation

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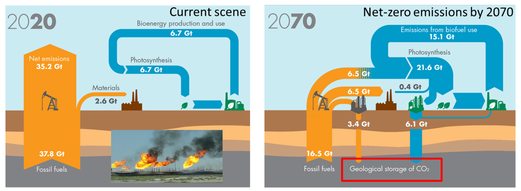
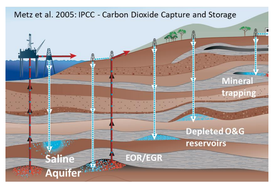
Motivation

Carbon Capture, Utilization and Storage (CCUS) is a key technology to overcome global warming caused by high GHG emissions. CO2 storage in geological formations is a highly recommended method for CO_2 sequestration.



Shell's Net Zero view

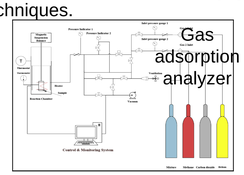


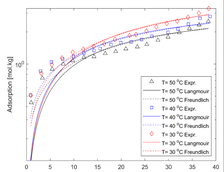
Including

- CCUS in coalbed to enhance methane recovery
- Unminable coalbeds at a deep location

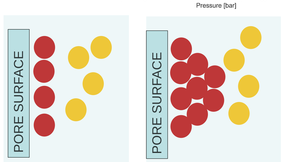
Gas adsorption on rock surface

CO_2 Adsorption on a solid surface is a **key storage mechanism** measured using gravimetric and volumetric lab techniques.





Thus, this work uses 1,064 data points to demonstrate ML application in predicting CO2 adsorption on coal surfaces.



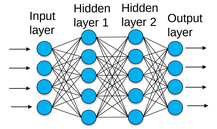
a) Monolayer Langmuir

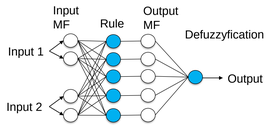
b) Multilayer BET

Methodology

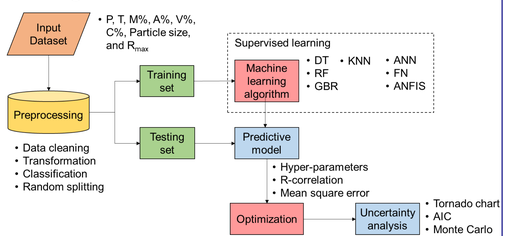
Machine learning tools

1. Decision Tree (DT)
2. Random Forest (RF)
3. Gradient Boost Regression (GBR)
4. K-nearest Neighbor (KNN)
5. Artificial Neural Network (ANN)
6. Function Network (FN)
7. Adaptive Neuro-Fuzzy Inference System (ANFIS)

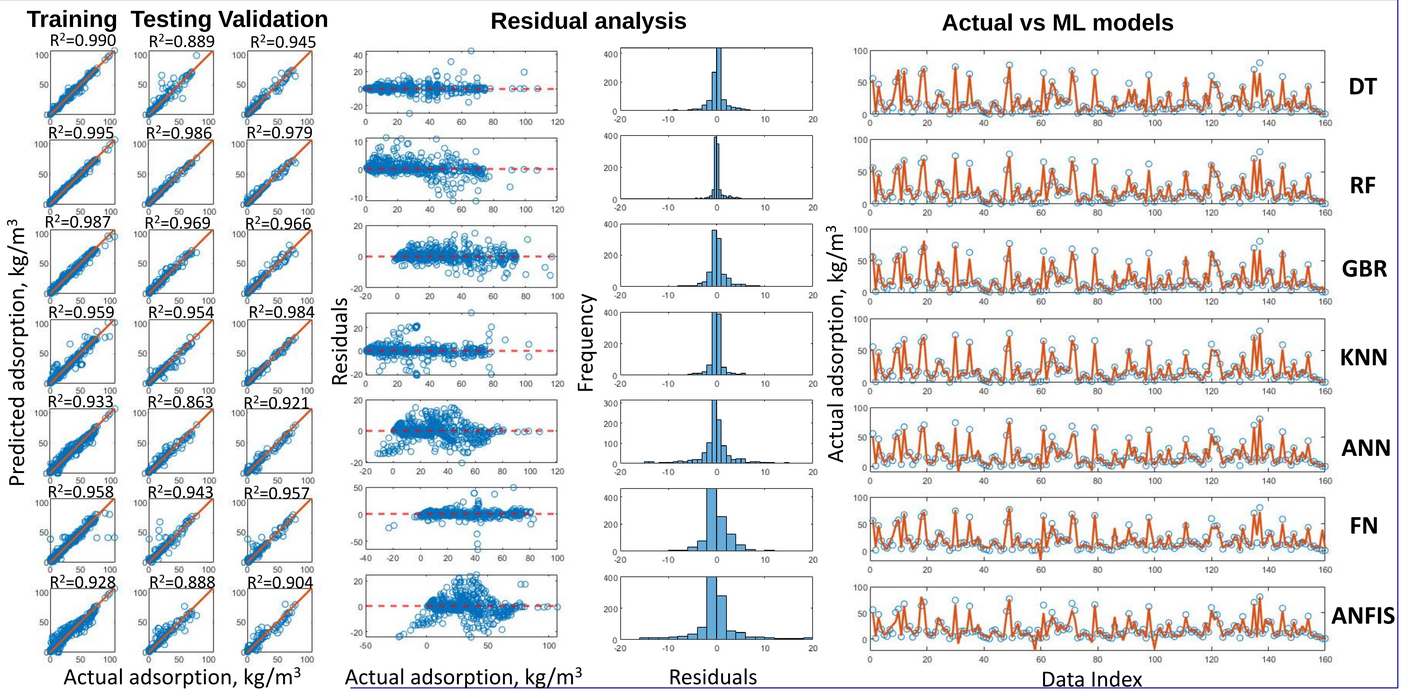




Modelling flowchart



Results

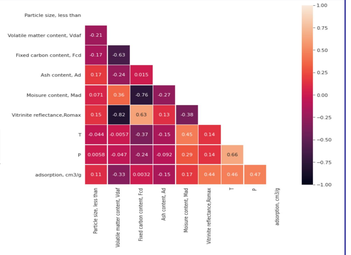


Data distribution

Correlation between parameters (input) and adsorption (output)

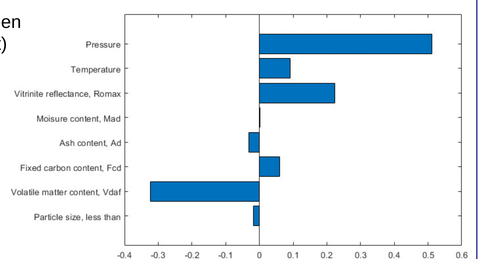
$$R = \frac{\left[\sum \frac{(x_i - \mu_x)(y_i - \mu_y)}{n-1}\right]}{\sigma_x \sigma_y}$$

- Pressure
- Temperature



Sensitivity & Uncertainty

Correlation between parameters (input) and adsorption (output)



Summary

Supervised machine learning can be applied to overcome mathematical models' deficiency and predict accurately the gas adsorption isotherms on a solid surface, as demonstrated by the CO_2 adsorption on coal prediction example in the present work.

References

Alanazi, A., Bawazeer, S., Ali, M., Keshavarz, A., Hoteit, H., 2022. Thermodynamic Modeling of Hydrogen-Water Systems with Gas Impurity at Various Conditions Using Cubic and PC-SAFT Equations of State. Energy Convers. Manag. X 100257. https://doi.org/10.1016/J.ECMX.2022.100257