Application of machine learning to develop a soft-sensor model for prediction of sorption-enhanced steam methane reforming performance

Paula Nkulikiyinka*; Peter Clough; Vasilije Manovic
Energy and Power Theme, School of Water, Energy and Environment,
Cranfield University, Cranfield, Bedfordshire, MK43 0AL, UK
* ***Email:*** *paula.nkulikiyinka@cranfield.ac.uk*

Hydrogen Production from Enhanced SMR

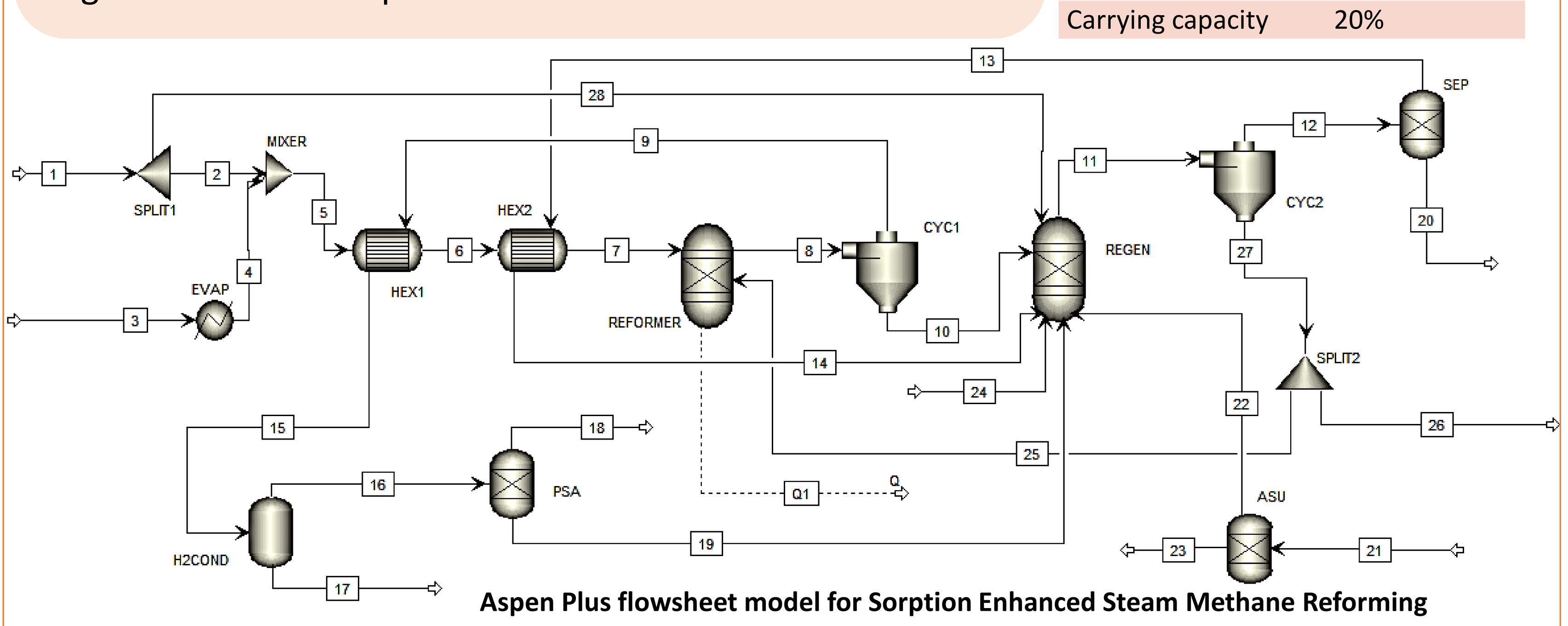
- **Hydrogen** is a highly sought after energy source as it can be produced in several ways & from numerous resources- both renewable and non-renewable. In addition, it's a **clean energy** source producing no greenhouse gases or other particulates, & is also a raw material for many eco-friendly and/or high efficiency power systems e.g. fuel cells [1].
- A popular H_2 production method is sorption enhanced steam methane reforming **(SE-SMR),** which encapsulates steam methane reforming with **calcium looping**; a CO_2 capture technology that uses CaO as a sorbent for **the capture of CO_2**
- Some constraints and limitations to **large scale hydrogen production** includes the high costs associated with the technology and hardware required to measure the progress of the process, as well as the physical inability to obtain certain measurements necessary for process control. A solution to this challenge, is the use of **soft sensors**, which are essentially inferential estimators [2][3].
- In recent years, **machine learning**, and in particular, soft sensors have been widely studied and used in other industrial processes such as process modelling and control of amine-based **post-combustion technology**, as well as other thermochemical processes, with the aim of **improving the quality** of product and **assuring safety** in production [4][5].
- Based on the dataset available and literature, two machine learning models have been used to develop a soft sensor model, in order to provide accurate prediction and estimation of variables that are otherwise unable to be accurately measured, using **artificial neural network (ANN)** and **random forest (RF)** algorithms.

Aspen Model for Enhanced SMR

Machine learning algorithms for the operation of the reactor have been developed firstly by modelling the process in **Aspen Plus**, with baseline conditions based on literature [6].

Then a **sensitivity analysis** was applied, in order to gather a large amount of data points.

Baseline Conditions	
S/C	4
Sorbent/C	1
Pressure	1 bar
Reformer	650°C
Regenerator	850°C
PSA efficiency	90%
Carrying capacity	20%



Aspen Plus flowsheet model for Sorption Enhanced Steam Methane Reforming

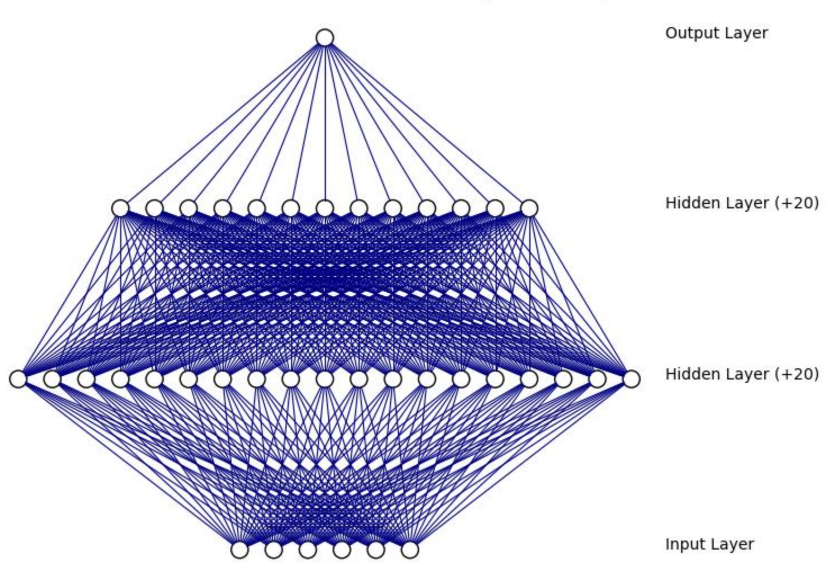
Streams	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28
CH_4	✓	✓			✓	✓	✓	neg.	neg.						neg.	neg.			neg.									✓
H2O			✓	✓	✓	✓	✓	✓	✓		✓	✓			✓	✓	✓		✓	✓								
CO								✓	✓		✓	✓			✓	✓			✓	✓								
CO_2								✓	✓		✓	✓	✓	✓	✓	✓			✓	✓								
H_2								✓	✓		✓	✓			✓	✓		✓	✓	✓								
CaO											✓														✓	✓	✓	
$CaCO_3$								✓		✓														✓				
O_2																					✓	✓						
N_2																					✓		✓					
Temp (°C)	25	25	25	150	123	400	477	650	650	650	850	850	850	497	420	25	25	25	25	850	25	25	25	25	850	850	850	25

Machine Learning Theory for Enhanced SMR

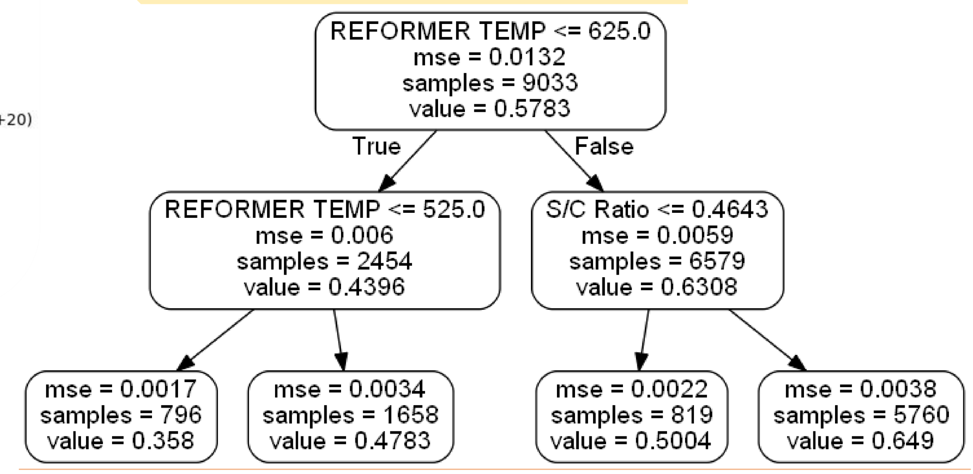
The data was then implemented into Python to predict the methane **conversion** and hydrogen **yield** and **purity** and **CO_2 capture efficiency.**

- CO_2 **Capture (%)** $= \frac{n_{CH_4,in} - n_{CH_4,out} - n_{CO_{out}} - n_{CO_{2,out}}}{n_{CH_4,in}} \times 100$
- H_2 **Purity (%)** $= \frac{n_{H_{2,out}}}{(n_{H_{2,out}} + n_{CH_{4,out}} + n_{CO_{out}} + n_{CO_{2,out}})} \times 100$
- **CH4 Conversion (%)** $= \frac{(n_{CH_4,in} - n_{CH_4,out})}{n_{CH_4,in}} \times 100$
- **H2 Yield (%)** $= \frac{n_{H_{2,out}}}{n_{H_{2,stoich}}} \times 100$

SE-SMR Neural Network architecture [6,39,33,1]



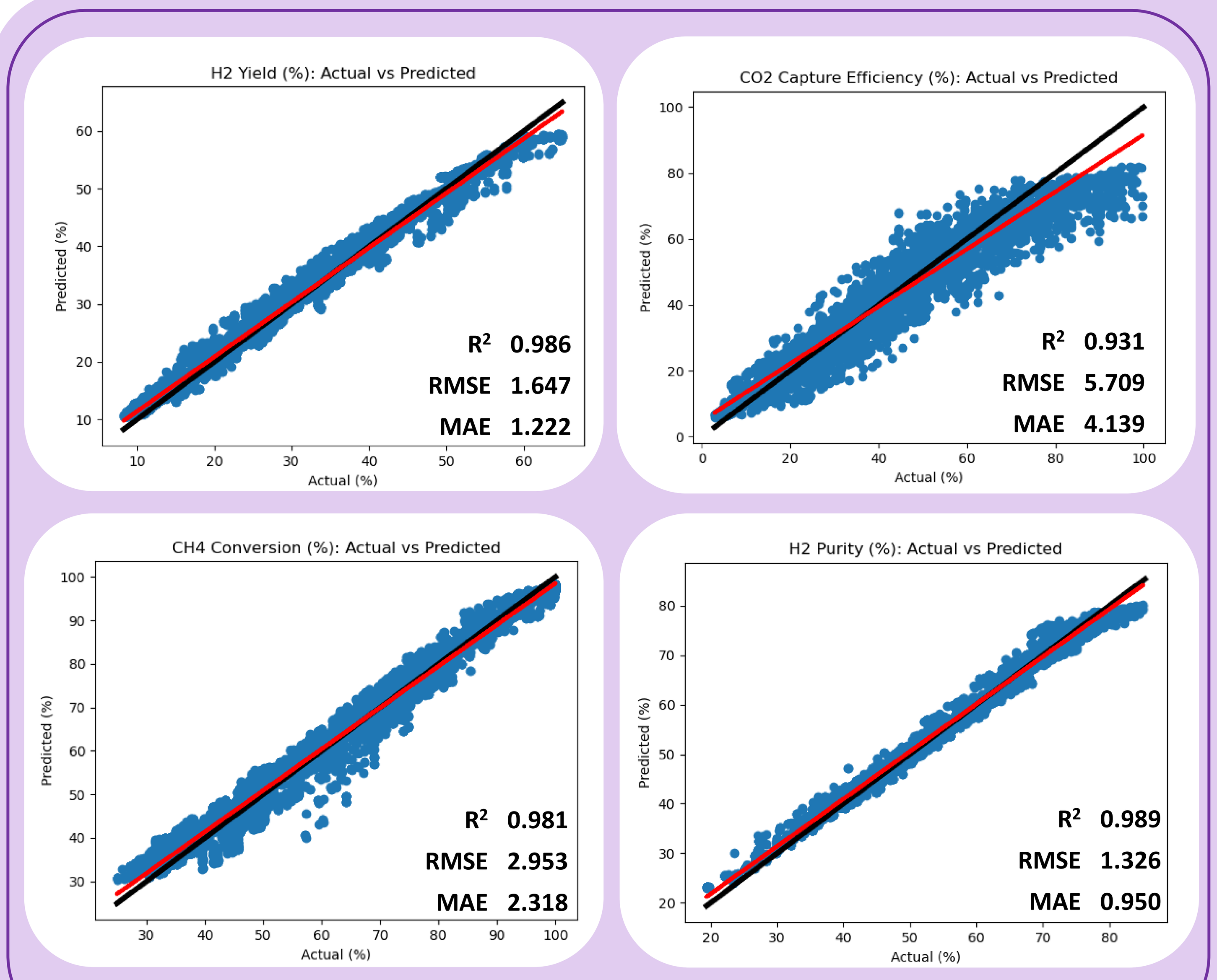
Left: The topology of the neural network with the configuration [6,39,33,1].



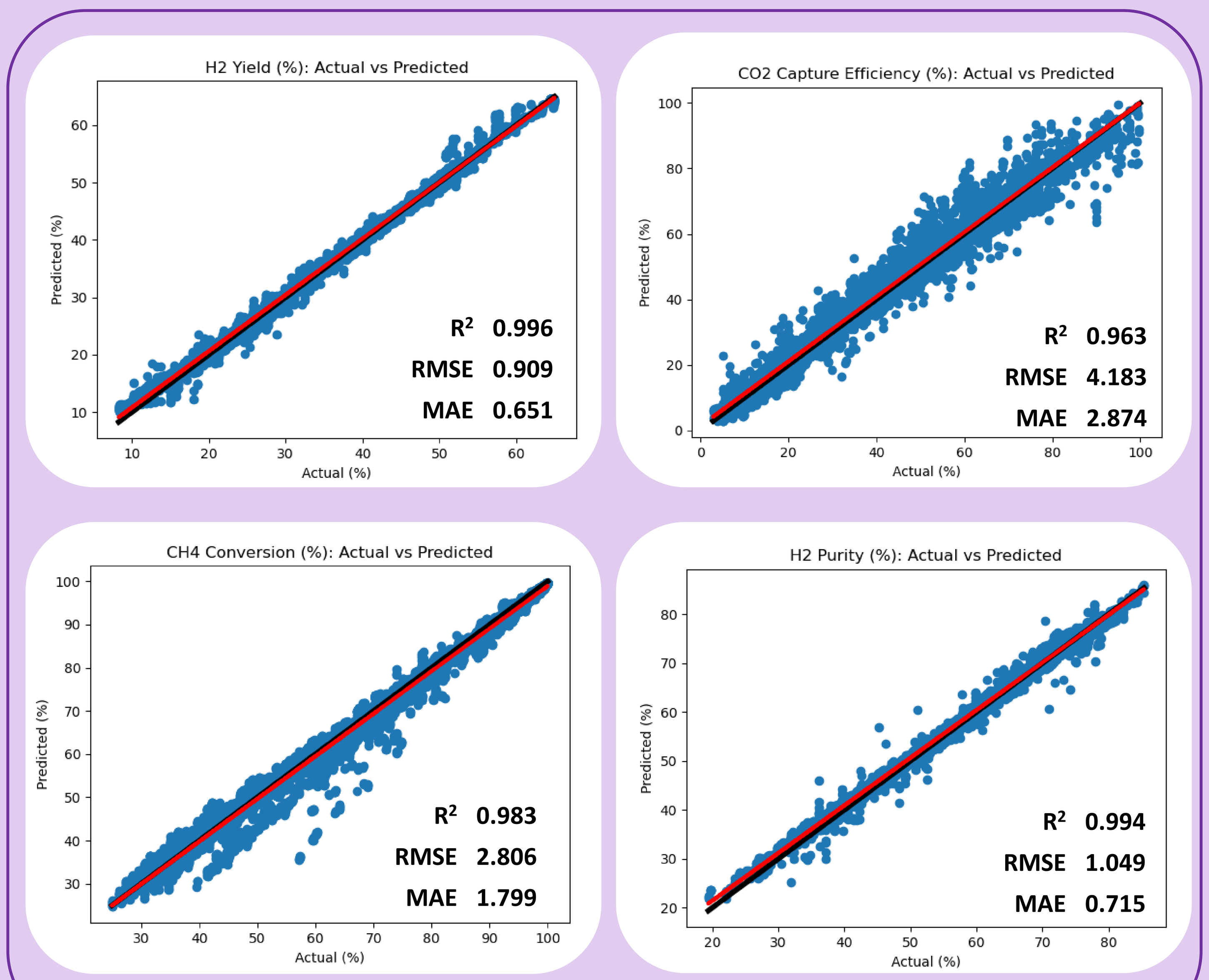
Right: An extract of 2 tree layers consisting of 'leaf nodes', number of samples split on the variable and the MSE value, in the Random Forest model

Machine Learning Results

- The Aspen input data (steam to carbon ratio, sorbent (CaO) to carbon ratio, reformer and regenerator temperatures and pressures) was plotted via Neural Network model and Random Trees Model, in Python language



Actual vs Predicted plot of CH_4 conversion, H_2 purity and H_2 yield modelled by random forest algorithm



Actual vs Predicted plot of CH_4 conversion, H_2 purity and H_2 yield modelled by neural network algorithm

- Obtained **Actual vs Predicted plot** for CH_4 conversion and H_2 yield and purity, as well as figures for CO_2 capture.

  Obtained accuracy metrics: mean square error **(MSE)**, mean absolute error **(MAE)**, mean absolute percentage error **(MAPE)**, Variable importance, R^2

  Confirmed the models were **consistent** with each other

Conclusion

- Both models are good predictors of output data, provided the input data is robust and there is a large quantity of training, testing and validation data
- The neural network model indicated higher levels of accuracy with higher R^2 values (0.96-0.99) and lower MAE (0.65-2.87) and RMSE (0.91-4.18) values compared to the random forest model: (0.93-0.98), (0.95-4.14) and (1.33-5.71) respectively.
- The developed models can easily be applied as a soft sensor for analysis and evaluation of a SE-SMR based hydrogen production plant to detect desired measurements

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