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Exploring predictive emissions monitoring of ammonia at TCM carbon-capture plant using open-source machine learning libraries

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Abstract

Carbon capture, utilisation and storage are critical mitigation pathways for decarbonising many industrial processes. The technology maturity, high capture efficiency, versatility and scalability continue to make amine-based carbon capture the leading technology. However, continuous improvement is required to overcome limitations and challenges associated with the technology. Process optimisation and solvent selection have helped reduce energy consumption and, thus, the carbon footprint. Material and solvent testing continues to help understand and mitigate corrosion and solvent degradation. This has led to measures that reduce equipment damage, solvent losses during operation and the environmental impact of solvent emissions and byproducts such as ammonia. Machine learning could potentially provide further insights.

The main objective of this paper is to explore the development of a predictive emissions monitoring system for ammonia using the open-source machine learning libraries Sci-kit Learn and the open-source programming language Python. The secondary objective is to identify the key operational parameters that significantly influence ammonia emissions.

Technology Centre Mongstad's (TCM) historical data from a data historian was extracted at five-minute intervals between 03-August-2015 and 13-September 2015. The data was collected during a baseline study using RFCC flue gas testing with MEA solvent. [1, 2]. The targeted ammonia emissions were monitored using a Gasmet FCX FTIR between 0- 500 ppm by volume measured on wet basis. A total of 75 input parameters from different operational units were evaluated. The operational units were divided into incoming flue gas, depleted flue gas, CO_2 product gas, Lean and rich amine, absorber, water wash, stripper, steam and condensate. All the identified input parameters had online measurements, which acquired data continuously and some were varied during plant operation. These are summarised in Table 1.

Data was processed by removing periods with plant stoppages, missing values, instrument errors and duplicate measurements. [3, 4] The correlation between the input parameters and ammonia emissions was evaluated using regression models. Four tree-based models (Decision Tree, Random Forest, Gradient Boosting, and lightGBM) and two traditional regression models (Linear regression and Support Vector Regression) were evaluated using 7,828 examples and tested with 3,355 examples. The tree-based regression models generally performed better than the linear-based models. Random Forest exhibited the best performance, with the lowest MSE (0.7040), RMSE (0.8390), MAE (0.2701), and the highest R^2 (0.9849).

Table 1: Input parameters that were explored

Operational unit	Process parameter
Incoming flue gas	Flow rate, pressure and temperature. Carbon dioxide, oxygen, water vapour, sulfur dioxide, ammonia and nitrogen concentration. Oxygen concentration
Depleted flue gas	Flow rate, pressure and temperature. Carbon dioxide concentration
CO_2 product gas	Flow rate, pressure and temperature. Carbon dioxide concentration
Lean and rich amine	Flow rate, temperature, density, conductivity and pH
Absorber	Temperature profile and level
Water washes	Flow rate, temperature, conductivity and pH
Stripper	Pressure and temperature
Steam & condensate	Flow rate, temperature and pressure

Table 2: Model performance comparison

Statistical test	Linear Regression	Decision Tree	Random Forest	Gradient Boosting	Support Vector Regression	LightGBM
MSE	3.6609	1.241	0.7283	1.3698	18.0665	1.0078
RMSE	1.9133	1.114	0.8534	1.1704	4.2505	1.0039
MAE	1.2473	0.3664	0.2716	0.623	0.8344	0.3833
R^2	0.9215	0.9734	0.9844	0.9706	0.6124	0.9784

A comparative assessment of the predicted versus measured value showed that most data was close to the perfect fit line, indicating a great match between the model's predictions and the actual value, as shown in Figure 1. Emissions trending showed that the model showed accurate predictive values during normal operation variation. The model was less accurate during abrupt increases or decreases in the measurements. Figure 2 shows that the prediction suffered when the measurement values were below the Limit of Detection (LOD) of the FTIR. The estimated LOD for ammonia was 1 ppmV.

At PCCC8, we will present our findings and lessons learnt from the exploratory study and discuss the process parameters that significantly impacted the prediction. The presentation will provide valuable insights to researchers, developers, and operators of amine-based carbon capture plants on the use of predictive machine learning algorithms in plant operations.

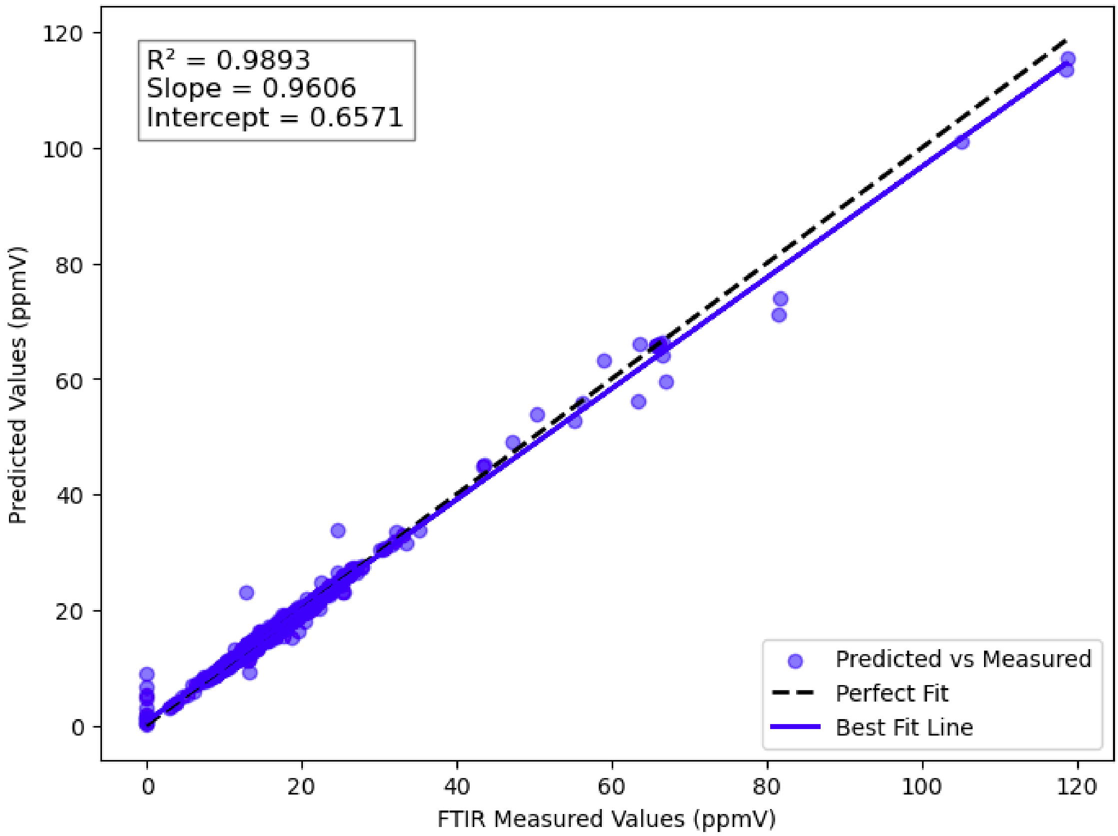

Figure 1: FTIR values versus predicted values. The blue solid line is the best fit regression line while the black dashed line is the 1:1 line.

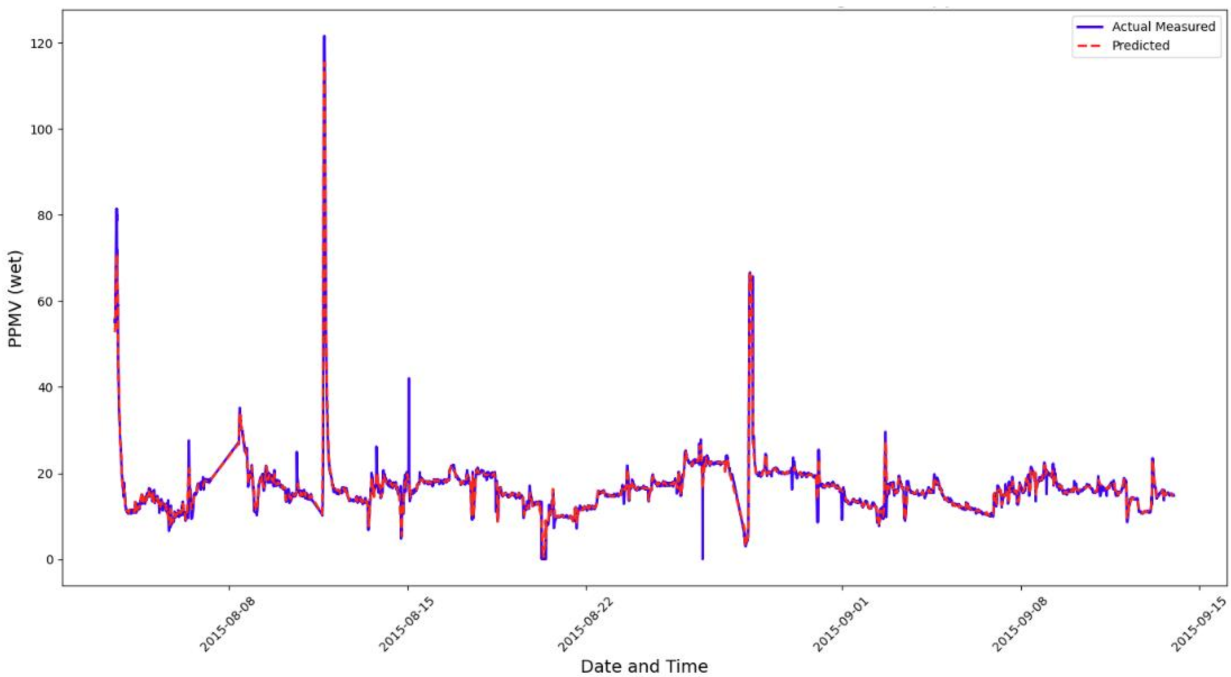

Figure 2: Time series of ammonia emissions from the FTIR compared to the predicted emissions using a Random Forest model

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Keywords: Predictive emissions monitoring; ammonia emissions; machine learning; regression models; flue gas; amine based carbon capture emissions, python, tree based ensemble, TCM, Technology Centre Mongstad.