



Optimizing Predictive Models for LNG Production and Temperature Forecasting

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ABSTRACT

Predicting LNG (Liquefied Natural Gas) production and associated rundown temperatures is crucial for efficient operations in the LNG industry. Accurate predictions enable better resource allocation, cost management, and maintenance planning. In this study, we compared the performance of various machine learning algorithms for their ability to forecast LNG production and rundown temperatures. We evaluated the predictions using error metrics, specifically the R2score and Root Mean Square Error (RMSE). The study revealed that the K-neighbors algorithm outperformed other models, exhibiting the highest R2 score and the lowest RMSE, making it the optimal choice for accurate predictions. Additionally, the feature selection process played a critical role in model accuracy, with certain features proving to be more suitable for training the models. Detailed error analysis and data visualization further demonstrated the effectiveness of the chosen algorithm. This study highlights the significance of selecting the right predictive model and features for LNG production and temperature forecasting, providing valuable insights for optimizing operations in the LNG industry.

Keywords: LNG Production Forecasting, Rundown Temperature Prediction, Machine Learning Algorithms, R2 Score Analysis, Root Mean Square Error (RMSE) Evaluation and KNeighbour

1. INTRODUCTION

The world is moving to natural gas from fossil fuels. Natural gas has supplanted coal as the world's cleanest and most ecologically friendly energy source due to its lower carbon emissions and affordability (Mofid & Fetanat, 2019; Salehi, 2018; Wang, 2017). Natural gas use is expected to rise 40% between 2014 and 2040. (BP, 2017). Jackson, Eiksund, and Brodal found that natural gas-powered plants provided 37% of fossil energy in 2030, up from 30% in 2013. (2017).

LNG is rapidly replacing fossil fuels as a key energy source worldwide because to its reduced greenhouse gas emissions and cleaner burning. These LNG benefits have attracted attention recently due to the energy crisis (Sang et al 2020). Natural gas is mostly transported via liquefaction and pipelines. Energy companies have routinely employed liquefying natural gas to transport it across long distances instead of pipes. The pipeline pressure difference limits pipeline gas supply, the transit route is rigid, and long-term contracts are needed (Lee et al 2020).

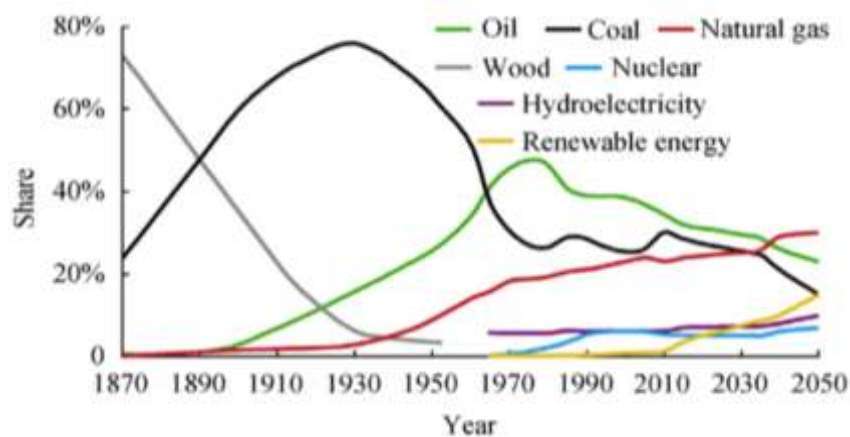


Figure 1. Global trend in energy consumption (U.S. Energy Information Administration, 2022)

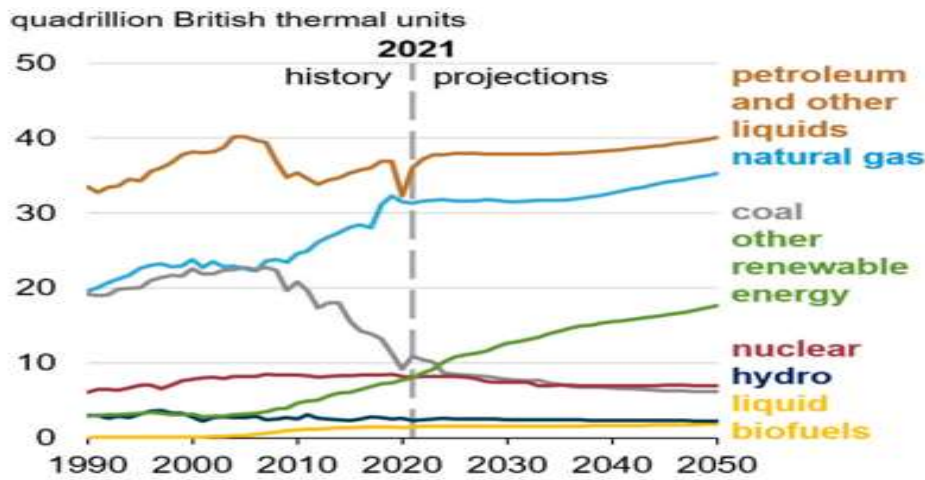


Figure 2. History and Projection of U.S. Energy Consumption (U.S. Energy Information Administration, 2022)

Liquefaction is the process by which gases are transformed into liquids. Liquefied natural gas (LNG) is natural gas that has been cooled to -162 degrees Celsius while maintaining an atmospheric pressure. Natural gas is more convenient to transport in this state since only one-six hundredth as much is utilized as when it is in its gaseous state (Khalilpour & Karima, 2009).

When temperatures drop below the critical temperature of natural gas, the gas changes phase and becomes a liquid. Refrigerants must be employed to reach such low temperatures, and the heating curves of these refrigerants must be as similar to the cooling curve of natural gas as is practically possible. A refrigerant is the fluid used to transport heat in air conditioning and refrigeration systems. Maintaining a cold temperature for the LNG product in LNG facilities is crucial for its storage and transport.

As a consequence, production will suffer if this section is inefficient. There is a need for environmentally friendly, fast-acting refrigerants that also save energy. Over the years, a number of distinct LNG production methods and refrigerant types have arisen, each with its own unique process configuration. Some examples are the turbo-expander process, the cascade process, and single/dual mixed refrigerant (SMR/DMR) technology. The primary distinctions between these methods are capital and operational costs. A company's capital expenditures (CAPEX) and operating expenditures (OPEX) are affected by a number of factors, including its production capacity, the quantity of equipment, and the cost of labor. However, the use of mixed-refrigerant (MR) processes greatly increases the complexity of process design and operation due to the increased number of thermodynamic interactions, making process management and optimization exceptionally challenging (Shukri, 2004). Factors like as desired temperature range, ease of access, cost, and past experience all factor into the decision of which refrigerant to use. Ethane and propane, for instance, may be on hand in a natural gas processing facility, whereas ethylene and propylene are on hand in an olefins factory. There is a substantial danger of contamination if propane or propylene were used in an ammonia facility, but ammonia might serve the same function. Due to their inability to catch fire, halocarbons have seen widespread use. The Propane Precooled Mixed Refrigerant (C3MR) system is one of the most popular refrigeration methods utilized today. Before entering the mixed refrigeration system consisting of methane, ethane, propane, and nitrogen, the liquefied natural gas is precooled to -35°C in a propane refrigeration system (Bahadori et al., 2014).

2.1 Methodology

2.1.1 Material

The material used in this research include: An artificial intelligent (Python programming language) software, PI Process book software 2015 version 3.6.2.271, PI datalink, Visual studio (VS) code editor and the Microsoft Excel 365. Python is an interpreted, high-level programming language that may be used for a wide variety of projects. The principle behind its design prioritizes the readability of the code by heavily indenting it. The PI process book and PI datalink add-in were basically used for data collection from the plant site. While the VS code editor is mainly an Integrated Development Environment (IDE) source code editor used to debug, highlight syntax and for coding of the GUI script. It is a user-friendly coding environment.

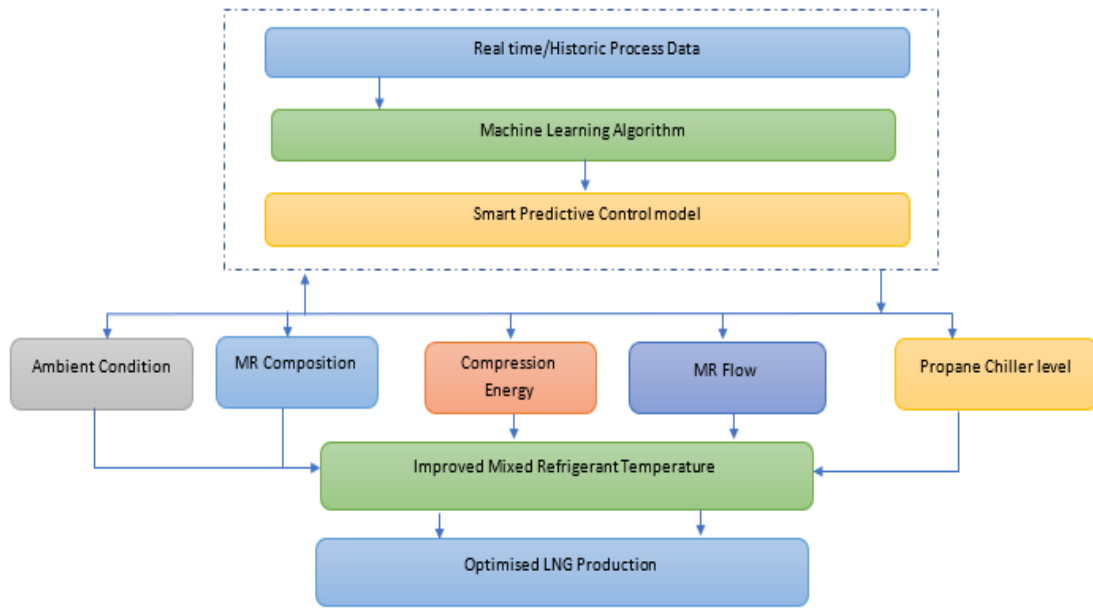


Figure 3. Research design framework for the optimization of LNG production using AI.

2.1.3 Process Optimization Description

Figure 4 shows the sequential order or steps used to achieve the aim and objectives of this research. It depicts the schematic breakdown of the optimization process using the artificial intelligence data driven approach.

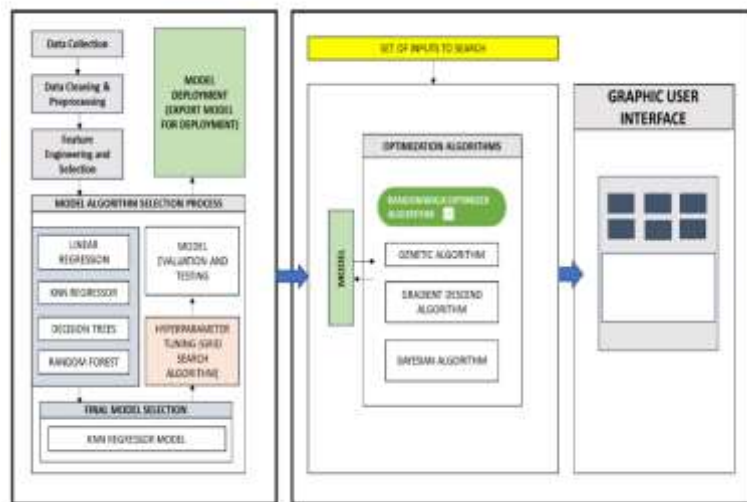


Figure 4. Process description of Artificial Intelligence optimisation

2.1.4 Data Collection

The data collection for this work was done using PI Processbook 2015 software version 3.6.2.271 R2 and PI datalink. PI processbook is an OSIsoft vendor software that enable users to retrieve real-time data from the PI system which is linked to a live process plant. The software application can create dynamical graphical display, trends from historical and real time data. To retrieve the data used for the work, the PI datalink was connected to the PI server and then to the liquefaction plant via several process control schemes as shown in figure 3.3. The PI datalink is a Microsoft Excel add-in feature

linked to the PI software. The PI datalink's sample data multiple value function was used to retrieve about 10 years liquefaction unit data set at an hourly interval.

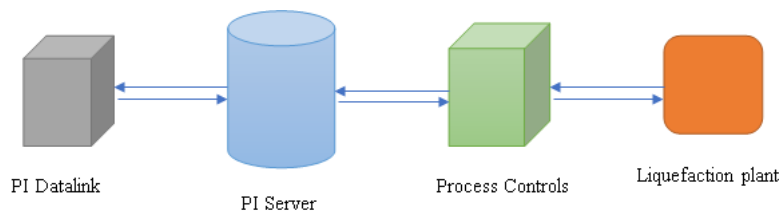


Figure 5. PI System data Collection scheme

2.1.5 Data Pre-processing and Cleaning

In this phase, three important steps were followed which are the data importation, cleaning of data, and exporting of data for next stage.

- **Importation of library and loading of data**

The data used for this project contains about 70,000 rows and 43 columns of about 10 years sample data. Microsoft excel was used to get a preview of how the data looks. The images below show the preview of the data in MS excel. The data seen above, as expected, contains quite a lot of invalid data and errors. Jupyter notebook version 6.4.5 environment was used, which comes as part of a software called Anaconda. Anaconda comes with a lot of libraries that will be so useful for me in this project. The first library that I used is the Pandas. Pandas with the help of python programming language was used to load the data into the Jupyter notebook environment. Below is the image that shows the data already imported into Jupyter notebook using Panda's python library. Figure 3.2 consist of data collected from the industry. Figure 3.3 displays the data loaded for the optimization process (first five rows of the data).

- **Cleaning the data.**

3. As mentioned earlier, the data loaded above contains many invalid inputs from the data collection source. Neglecting these errors will lead to making an inaccurate model. Hence, there is need for me to handle and get rid of them. These involve creating the data in a floating type. Data cleansing involved the following processes.

- i. Eliminated erratic values in LNG flow column.
- ii. Found out the error values in "MCHE cold bundle dp" column.
- iii. Found out the errors in "volumetric MR flow to MR component discharge" column.
- iv. Found out errors in "percentage Nitrogen in MR" column.
- v. Removed unnamed columns.
- vi. Eliminated all the null values.

LNG Flow	SNG Shutdown Temperature	MR Operating Margin	MR Operating Margin	MR Compressor Outlet Pressure	MCHE Warm System Temperature	MR Inlet Temperature	MR Compressor Inlet Temperature	MR Inlet Temp Tag	MR Inlet Valve Opening	MR Inlet Valve	MCHE Cold Bundle dp	MR Flow to Discharge	MR Flow
12096.0438	189.8203	2.0396	18.2996	2.3178	-41.9019	-38.9896	-127.8699	4.4038	30.3384	159.7271	MR Data	MR Data	
12095.9419	189.8206	2.0213	18.2273	2.3271	-41.9249	-37.9332	-127.8072	4.4095	32.4768	169.8238	MR Data	MR Data	
12116.1689	189.8206	2.1083	19.0399	2.3297	-42.4023	-37.9753	-127.4081	4.4153	32.0188	169.3258	MR Data	MR Data	
12121.3887	189.8202	2.0866	19.6399	2.3471	-42.7085	-37.7172	-127.2754	4.4157	34.9384	184.3478	MR Data	MR Data	
12091.2441	189.8496	2.0191	18.8399	2.3412	-42.9981	-37.9891	-127.2618	4.3996	36.7162	181.7129	MR Data	MR Data	
12050.2088	189.8204	2.0815	20.4161	2.3418	-42.9168	-37.9172	-127.2714	4.4041	36.9963	184.2612	MR Data	MR Data	
12062.6191	189.8206	2.1345	20.7899	2.3338	-42.2412	-37.1267	-127.3238	4.4118	35.9445	184.7579	MR Data	MR Data	
12147.3164	189.8356	2.1216	21.1991	2.3222	-41.9482	-37.1827	-127.3438	4.4096	34.8732	180.8108	MR Data	MR Data	
12169.7071	189.8691	2.0869	20.7897	2.3271	-42.9828	-37.1641	-127.3121	4.4238	39.0799	182.9769	MR Data	MR Data	
11997.9127	189.8496	2.0782	19.7899	2.3174	-41.9174	-38.9946	-127.3729	4.4192	32.4715	182.8812	MR Data	MR Data	
12116.8945	189.8927	2.0112	17.6399	2.3068	-41.8838	-38.9219	-127.4982	4.4711	32.9299	189.8291	MR Data	MR Data	
12091.2168	189.7764	2.1739	19.8799	2.3844	-42.9186	-38.8395	-129.4762	4.4986	71.8889	153.3099	MR Data	MR Data	
11757.0439	189.8928	2.1844	7.1357	2.3034	-41.9634	-38.8682	-129.3887	4.4916	69.9213	148.3259	MR Data	MR Data	
11836.9073	189.8928	2.0853	8.4434	2.2799	-41.9898	-38.3329	-130.5428	4.4320	62.9068	142.7291	MR Data	MR Data	
11853.0523	189.8398	2.0199	3.8950	2.2754	-41.9992	-38.1290	-129.7482	4.4555	67.6188	143.9378	MR Data	MR Data	
11412.8973	189.8799	2.0979	3.5490	2.2771	-41.9122	-38.8872	-129.7389	4.4999	69.9448	142.8888	MR Data	MR Data	
11897.7688	189.7910	2.0198	4.8482	2.2963	-42.9281	-38.9699	-129.9991	4.4926	66.7181	121.8469	MR Data	MR Data	
11611.6694	189.8923	2.1454	4.9865	2.3059	-42.9599	-38.4877	-129.9999	4.4369	70.5979	143.4315	MR Data	MR Data	
11862.7079	189.8203	2.1673	8.0787	2.3268	-41.8778	-38.6889	-129.3262	4.3662	73.7359	152.8078	MR Data	MR Data	
11989.2012	189.8203	2.4626	8.3824	2.3244	-42.9897	-38.1976	-129.7169	4.3799	71.6249	141.1963	MR Data	MR Data	
11899.3452	189.8204	2.1189	6.0919	2.2744	-41.8974	-38.9423	-129.2012	4.4871	70.9294	155.1239	MR Data	MR Data	
11973.4482	189.8496	2.0888	7.3199	2.3084	-42.2383	-38.2852	-129.1201	4.4531	77.7747	147.9844	MR Data	MR Data	
11826.8168	189.8306	2.0874	7.7399	2.2732	-41.9922	-38.2221	-127.8982	4.4502	82.9942	146.8172	MR Data	MR Data	
11771.9646	189.8924	2.1841	8.1891	2.2943	-42.3936	-38.4435	-127.9064	4.4664	86.9453	156.3729	MR Data	MR Data	
11756.6248	189.7636	2.0172	6.7434	2.3068	-41.9164	-38.6993	-130.9614	4.4531	77.2671	144.8869	MR Data	MR Data	
11772.5742	189.8496	2.3095	7.0590	2.3813	-42.6045	-38.1839	-129.4298	4.3262	77.0989	153.3291	MR Data	MR Data	
11807.3281	189.7910	2.0388	5.9999	2.3162	-41.9612	-38.9695	-129.2011	4.4309	73.3227	149.3206	MR Data	MR Data	
11951.3489	189.8926	2.0919	3.1899	2.3059	-42.9291	-38.1792	-129.8782	4.3694	75.1939	159.4953	MR Data	MR Data	
11796.2891	189.8348	2.4414	8.9472	2.3511	-42.2622	-38.3989	-127.7579	4.3994	89.9989	159.9953	MR Data	MR Data	

Figure 5. Data library from Microsoft Excel

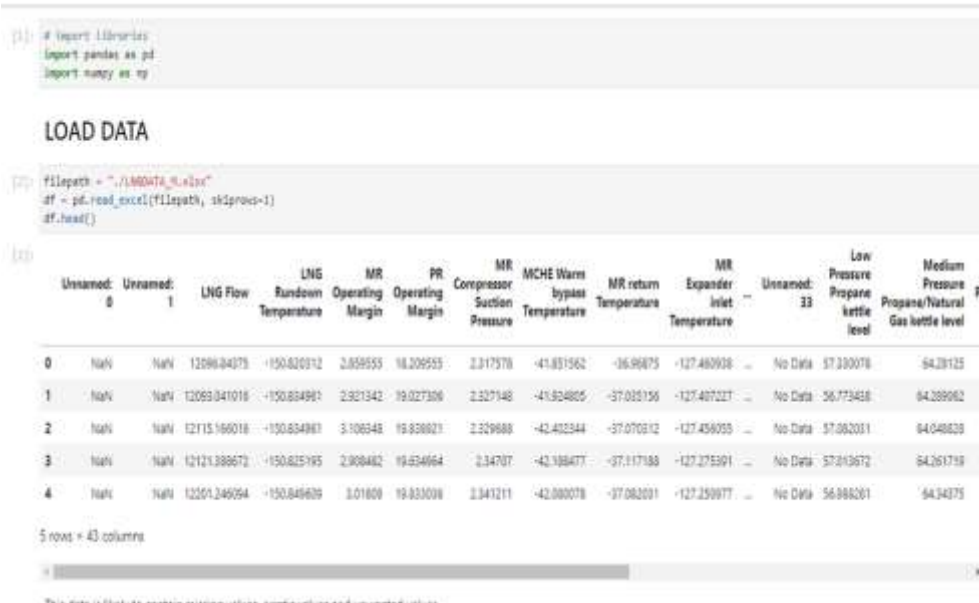


Figure 6 Previewed data for optimization process.



Figure 7. LNG data before cleaning

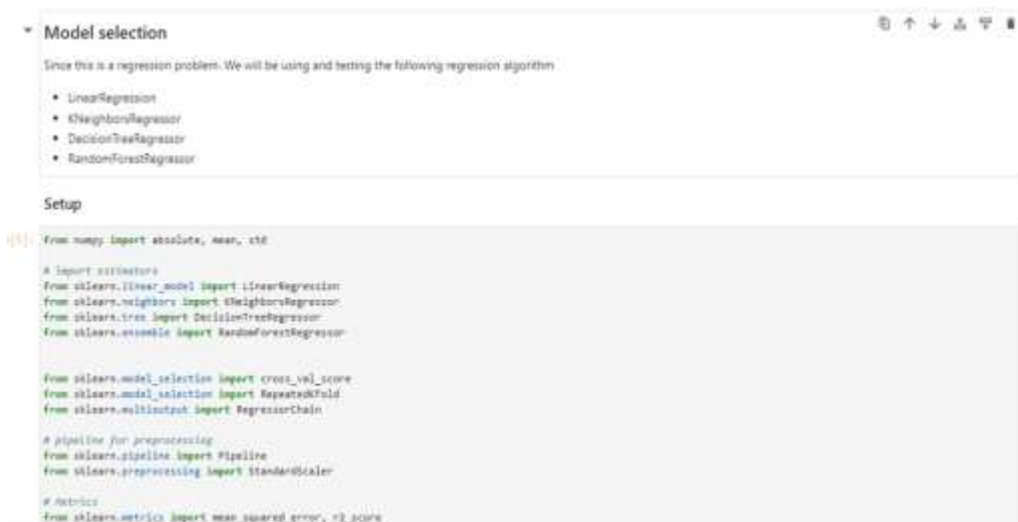
0	LNG Flow	32024 non-null	float64
1	LNG Rundown Temperature	32024 non-null	float64
2	MR Operating Margin	32024 non-null	float64
3	PR Operating Margin	32024 non-null	float64
4	MR Compressor Suction Pressure	32024 non-null	float64
5	MCHE Warm bypass Temperature	32024 non-null	float64
6	MR return Temperature	32024 non-null	float64
7	MR Expander inlet Temperature	32024 non-null	float64
8	LNG Shell Temp Top Bundle	32024 non-null	float64
9	LMR JT Valve Valve Opening	32024 non-null	float64
10	MCHE Cold bundle dp	32024 non-null	float64
11	Volumetric MR Flow to MR comp. discharge	32024 non-null	float64
12	HMR Flow	32024 non-null	float64
13	HMR/MR Ratio	32024 non-null	float64
14	LNG Flow Ex MCHE	32024 non-null	float64
15	MCHE Warm Bypass Temperature	32024 non-null	float64
16	MR IGV Position	32024 non-null	float64
17	MR Vessel Level	32024 non-null	float64
18	MR Vessel Pressure	32024 non-null	float64
19	Percentage Nitrogen in MR	32024 non-null	float64
20	Percentage Methane in MR	32024 non-null	float64
21	Percentage Ethane in MR	32024 non-null	float64
22	Percentage Propane in MR	32024 non-null	float64
23	Percentage Butane in MR	32024 non-null	float64
24	Nitrogen Make-up flow	32024 non-null	float64
25	Methane Make-up flow	32024 non-null	float64
26	Ethane Make-up flow	32024 non-null	float64
27	Propane Make-up flow	32024 non-null	float64
28	Ambient Condition	32024 non-null	float64
29	Scrub Column inlet Temperature	32024 non-null	float64
30	Natural Gas temp at MCHE warm bundle	32024 non-null	float64
31	Low Pressure Propane kettle level	32024 non-null	float64
32	Medium Pressure Propane/Natural Gas kettle level	32024 non-null	float64

Figure 8 LNG data after cleansing showing floating columns.

2.1.6 Model Selection Process

Several algorithms were tested on the two data set generated to determine the best LNG production and LNG temperature. In this process, LNG production (Uni-output) and LNG production and LNG rundown temperature (multi-output) were predicted. The data set up were loaded alongside the pandas, numpy and sklearn libraries. List of libraries and function loaded are listed below viz:

- Functions for calculating absolute, mean and standard deviation from the Numpy library
- Algorithm program from the sklearn library
- Programs chaining the algorithm available from the sklearn library
- Programs to process the data to make them suitable for the algorithm to work with
- Programs for metric calculations



```

Model selection
Since this is a regression problem, we will be using and testing the following regression algorithms:
• LinearRegression
• KNeighborsRegressor
• DecisionTreeRegressor
• RandomForestRegressor

Setup
In [1]: from numpy import absolute, mean, std

# Import structure
from sklearn.linear_model import LinearRegression
from sklearn.neighbors import KNeighborsRegressor
from sklearn.tree import DecisionTreeRegressor
from sklearn.ensemble import RandomForestRegressor

from sklearn.model_selection import cross_val_score
from sklearn.model_selection import RepeatedKFold
from sklearn.pipeline import Pipeline

# pipeline for preprocessing
from sklearn.pipeline import Pipeline
from sklearn.preprocessing import StandardScaler

# Metrics
from sklearn.metrics import mean_squared_error, r2_score

```

Figure 91 Library importation for algorithmic process

The following algorithms were imported:

- Linear Regression
- KNeighbors Regressor
- Decision Tree Regressor
- Random Forest Regressor

These algorithms are considered fit for the nature of task to be solved. This task is a numerical input, continuous target problem. It is numerical input because all our input features are of numeric datatype, and it is continuous (or numerical) target because the variables that I intend to predict are also numeric in nature.

- **Linear Regression**

The multiple linear regression model was used in the process due to several independent variables. The underlying equation for the multiple linear regression.

$$\beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_p x_p + \epsilon \quad \text{Equation 1}$$

- y_i is the dependent or predicted variable
- β_0 is the y-intercept.
- β_i are the regression coefficients representing the change in y relative to a one-unit change in x_1, x_2, \dots, x_p respectively.
- β_p is the slope coefficient for each independent variable
- ϵ is the model's random error (residual) term.

The cost function provides the best possible values for $\beta_0, \beta_1, \beta_2, \dots, \beta_p$ to make the best fit line for the data points. The algorithm converts this problem into a minimization problem to get the best values for β . The error is minimized in this problem between the actual value and the predicted value.

$$\text{minimize } \frac{1}{n} \sum_{i=1}^n (\text{pred}_i - y_i)^2 \quad \text{Equation 2}$$

$$J = \frac{1}{n} \sum_{i=1}^n (\text{pred}_i - y_i)^2 \quad \text{Equation 3}$$

- **KNeighbors Regressor**

The straightforward algorithm K nearest neighbors predicts the numerical target based on a similarity metric while storing all of the available cases (e.g., distance functions).

Distance function

$$\text{Euclidean } \sqrt{\sum_{i=1}^k (x_i - y_i)^2} \quad \text{Equation 4}$$

$$\text{Manhattan } \sum_{i=1}^k |x_i - y_i| \quad \text{Equation 5}$$

$$\text{Minkowski } (\sum_{i=0}^n (|x_i - y_i|)^q)^{\frac{1}{q}}$$

Equation 6

2.1.6 Model Development

The algorithm with more acceptable metrics from the model evaluation was selected.

This works best for the prediction to be performed. The following steps were used to prepare the machine learning model and load library dataset and the useful libraries model.

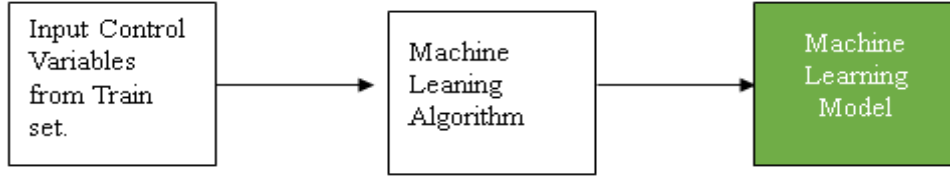


Figure 10. Flow chart for Model Development

The KNN algorithm was used to train the model.

Model Testing and Input Optimisation Using Optimisation Algorithms

The model was combined with several optimization algorithm on new set of inputs from another LNG plant data. The optimisation algorithm uses the model to find the best control variables or set points that will give an optimised LNG flow is shown below. Then compared with the new result.

The diagram below shows the model testing algorithm.

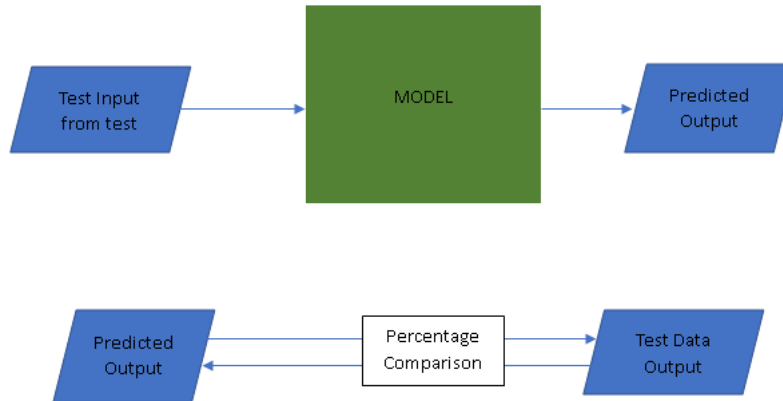


Figure 11. Model testing algorithm flow chart

3.0 Result and Discussion

3.1 Model performance (Kneighbor Regressor)

Table 4. 1 Error analysis of algorithms

S/No	Algorithm	R2 - Score	RMSE
1.	Linear Regressor	0.9411	628.9384
2.	K-neighbors	0.9853	313.8738
3.	Decision Tree	0.9748	411.4508
4.	Random Forest	0.8981	826.8076

Table 2. Error Analysis on the Algorithm performance for the actual LNG flow and actual LNG Rundown temperature

Data Row No	Actual LNG Flow	Actual LNG Rundown Temperature
18778	13575.379883	-145.473633
10519	11672.666016	-145.039062
31757	13300.155273	-145.786133
6400	12687.996094	-145.610352
17354	11994.082031	-145.502930

Table 3 Error Analysis on Algorithm performance for the Predicted LNG flow and predicted LNG Rundown temperature

Data Row No	Predicted LNG Flow	Predicted LNG Rundown Temperature
0	13363.826953	-146.179688
1	12060.130078	-145.521484
2	13391.834180	-145.701172
3	12811.619531	-145.620117
4	11980.771289	-145.903320

Table 4 Comparison of predicted and actual LNG flow using the K-Neighbor regressor Model.

Actual LNG Flow	Predicted LNG Flow	Error
13575.3799	13363.8269	211.553
11672.66	12060.1301	387.4641
13388.1553	13391.8341	3.6788
12687.9961	12811.6195	123.6234
11994.082	11980.7713	13.3107
Actual Rundown Temperature (°C)	Predicted Rundown Temperature (°C)	Error
-145.4736	-146.1797	0.7061
-145.0391	-145.5215	0.4824
-145.7861	-145.7012	0.0849
-145.6104	-145.6201	0.0097
-145.5029	-145.9033	0.4004

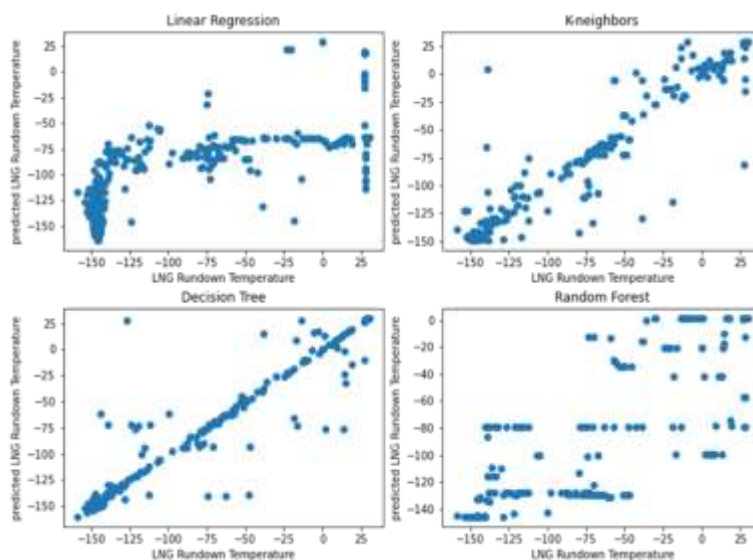


Figure 12. LNG Rundown Temperature Prediction

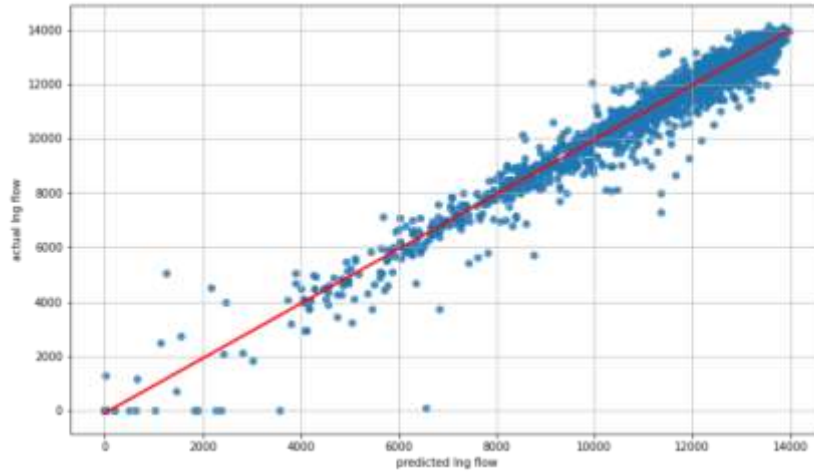


Figure 13. Final Visualization of Algorithm performance (actual LNG flow)

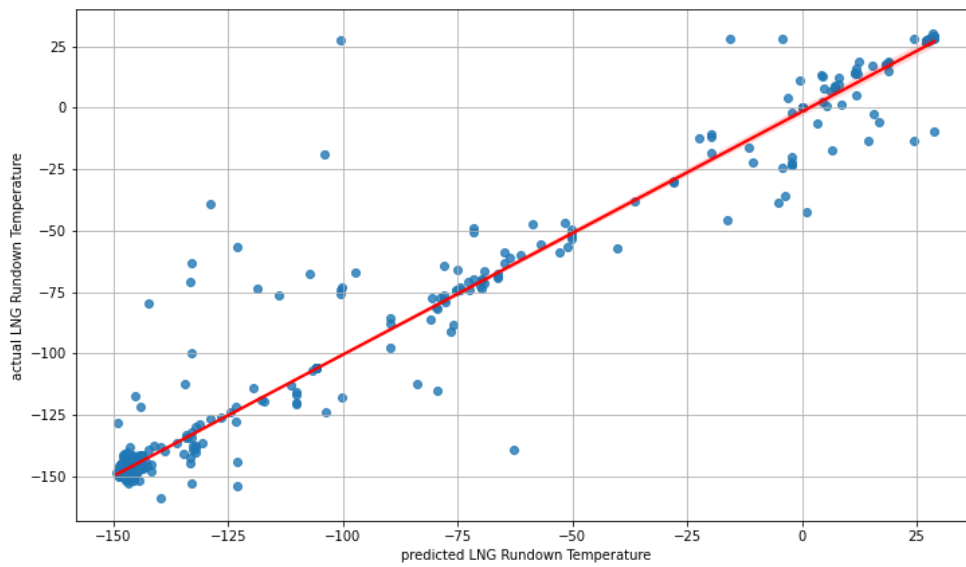


Figure 14. Final Visualization of Algorithm performance (LNG rundown temperature)

Table 5.. Improved prediction after hyper parameter tuning.

Data Row No	Predicted LNG Flow	Predicted LNG Rundown Temperature
0	13509.923222	-145.550721
1	12170.430456	-145.727184
2	13404.951410	-145.707795
3	12735.611069	-145.785677
4	11952.358026	-146.056697

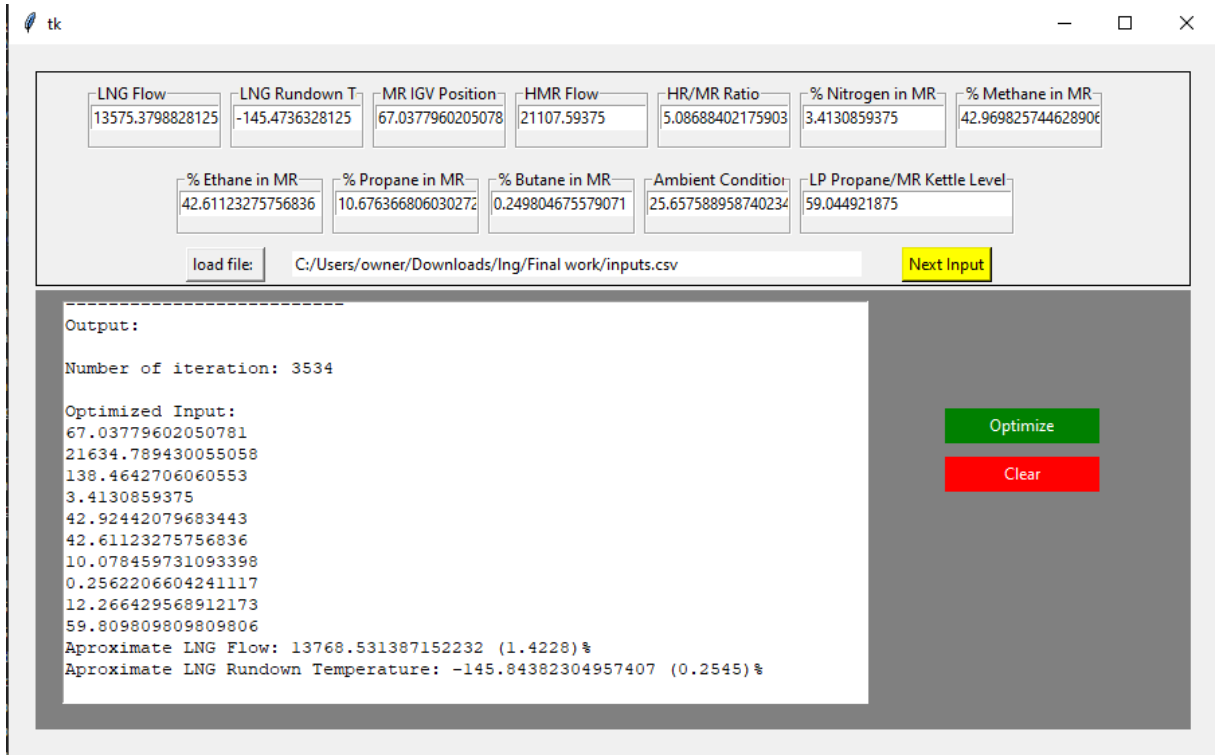


Figure 15. GUI run test 1

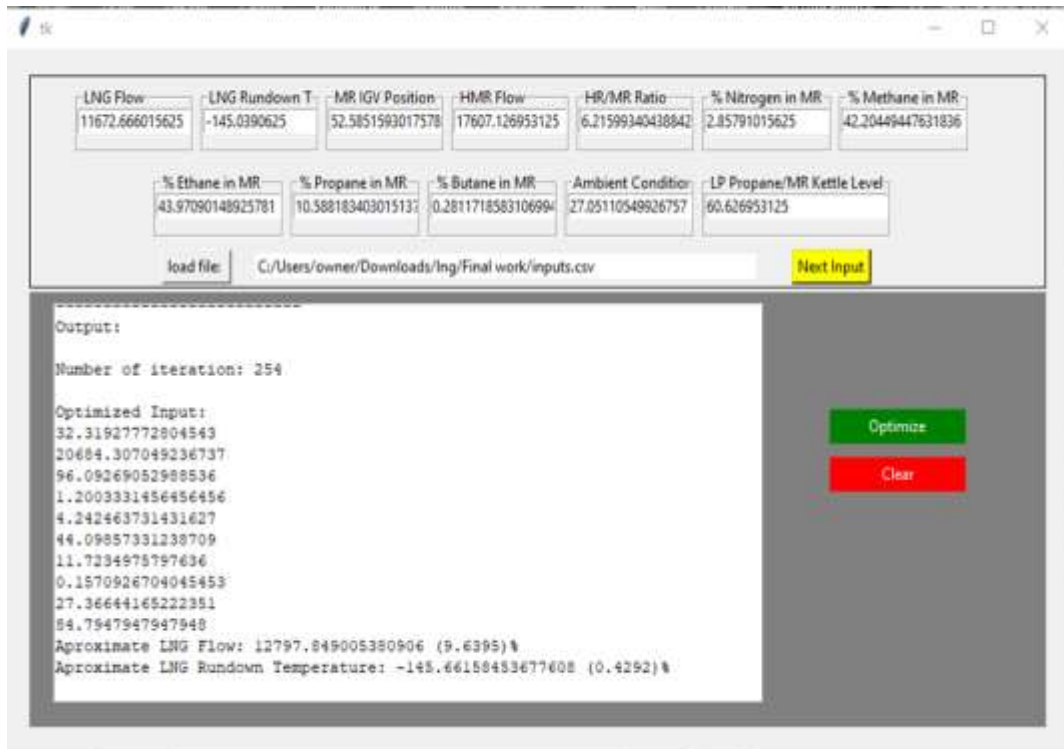


Figure 16. GUI run test 2

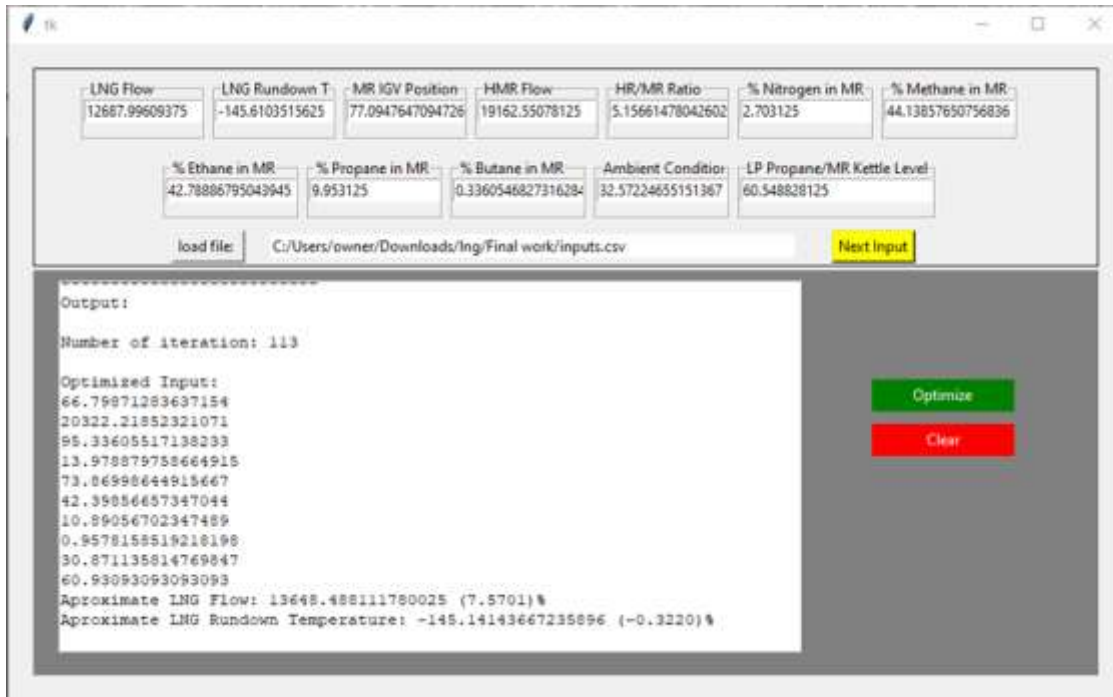


Figure 17. GUI run test 3



Figure 18. relationship between predicted and actual LNG flow

Table 6. Improved prediction for hyperparameter tuning.

Actual LNG Flow	Predicted LNG Flow	Error
13575.3799	13509.9223	65.458
11672.66	12170.4305	497.7645
13388.1553	13404.9514	16.7961
12687.9961	12735.6111	47.615
11994.082	11952.358	41.724
Actual Rundown Temperature (°C)	Predicted Rundown Temperature (°C)	Error
-145.4736	-145.5507	0.07061
-145.0391	-145.7272	0.6881
-145.7861	-145.7077	0.0784
-145.6104	-145.7856	0.1752
-145.5029	-146.0567	0.5538

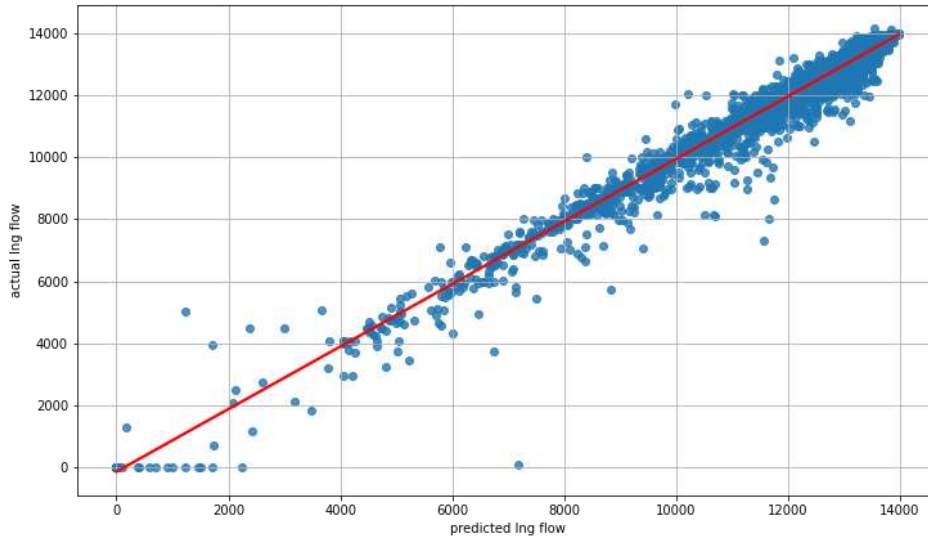


Figure 18. Visualization of Algorithm performance (based on LNG flow)

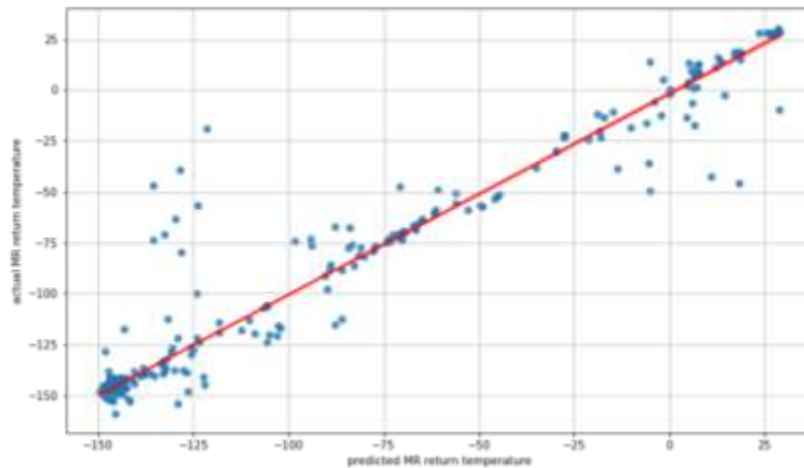


Figure 15. Visualization of Algorithm performance (based MR return and predicted temperature)

3.2 Discussion

To interpret the algorithm results, we compare the errors (R2 error and Root Mean Square Error (RMSE)). A good prediction should have a high R2_score (range between 0 to 1) and a low RMSE. The RMSE has to be as low as possible. The lower the RMSE, the more accurate the prediction. The goal here is to determine which of the algorithms will give the best R2_score and RMSE. The algorithms were trained with the train dataset command that was selected by intuition to learn how to predict LNG production (uni-output regressor). It was deduced that all the different algorithms' predictions had very good R2 scores. The K-neighbours algorithm gave the best regressor, with an R2 score of 0.9853, followed by the decision tree, whose R2 score was 0.9748, and the linear regressor, whose score was 0.9411. Although still a very good score, Random Forest had the lowest R2 score of 0.8981 amongst the other algorithms. Observing the RMSE metrics, it can also be seen that the K-neighbours had the lowest error in their prediction compared to the others. The RMSE of K-neighbours was 313.8738, and the Decision Tree came closest with an error of 414.4508.

Comparing Figure 12 and Figure 14, we see that the features chosen by intuition serve as the best to train and build the model for predicting LNG production and LNG rundown temperature. From the figures, we chose K-neighbours because it gave the best R2-score and the lowest RMSE. Figure 15 shows the actual part of the output in the test dataset, while Figure 16 shows the predicted output in the test dataset from the K-neighbour regressor model.

Using K-Neighbours, the actual LNG flow and rundown temperatures were compared to what was predicted, and the errors were also calculated. The lowest error (3.6788) was computed when the flow of the LNG was 13388.1553 and the predicted flow was 13391.8341; next to the actual flow of 11994.082 and a predicted flow of 11980.7713; the error computed by the K-neighbours was 13.3107. The corresponding temperatures are (-145.7861 and -145.7012; -145.5029 and -145.9033) while the errors are 0.0849 and 0.4004 See Table 1 above. Figure 17 and Figure 18 show the scatter plot representing the relationship between the actual output and the predicted output of LNG production and LNG rundown temperatures, respectively. We

observe a sharper, high-positive correlation in Figure 18, which explains that the difference between the actual LNG production and predicted LNG production is close and within an acceptable range.

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