National College of Ireland

Configuration Manual

MSc AI for Business
Practicum 2

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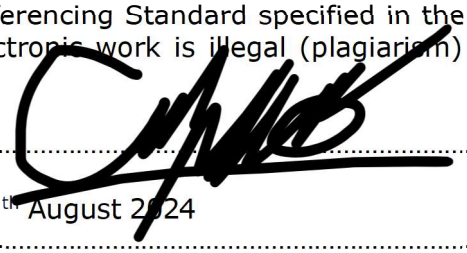
MSc AI for Business

Project Submission Sheet

School of Computing

Student Name:	Cristóbal Cáceres Ortúzar
Student ID:	23425849
Programme:	Ai For Business **Year:** 2024 - 2025
Module:	Practicum 2
Lecturer:	Dr Muslim Jameel Syed
Submission Due Date:	11th August 2024
Project Title:	Optimizing Green Hydrogen Production: An AI-Based Approach
Word Count:	xxx **Page Count:** 15

I hereby certify that the information contained in this (my submission) is information pertaining to research I conducted for this project. All information other than my own contribution will be fully referenced and listed in the relevant bibliography section at the rear of the project.
ALL internet material must be referenced in the bibliography section. Students are required to use the Referencing Standard specified in the report template. To use other author's written or electronic work is illegal (plagiarism) and may result in disciplinary action.

Signature: 

Date: 11th August 2024

PLEASE READ THE FOLLOWING INSTRUCTIONS AND CHECKLIST

Attach a completed copy of this sheet to each project (including multiple copies)	□
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Assignments that are submitted to the Programme Coordinator Office must be placed into the assignment box located outside the office.

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Signature:	
Date:	
Penalty Applied (if applicable):	

Configuration Manual

Cristóbal Cáceres Ortúzar

Student ID: 23425849

1. System Requirements

RAM: 16GB
OS: Windows 10
Processor: intel evo i7 g
Technology required: Python

The project needs Python 3.10+ along with Jupyter Notebook or Google Colab for execution.
Main Libraries: pandas, numpy, matplotlib, seaborn, scikit-learn, skopt, shap, joblib, statsmodels

2. Essential Steps to Follow

Step 1: Data Loading

The renewable_hydrogen_dataset_2535.csv file was accessed by Pandas. The file contains 2,535 entries where multiple independent variables like solar and wind power along with electrolyzer features and environmental parameters match with the target variable Hydrogen_Production_kg/day. The data gets loaded into a DataFrame which provides high-speed operations for modification and statistical analysis before ML integration. (Urhan et al., 2025; Naveena et al., 2024).

Step 2: Data Preprocessing

The model required numerical data so all non-numerical entries were discarded. The independent variables (X) received separate treatment from the dependent variable (y) that measured hydrogen production on a daily basis. The correlation matrix displayed variable relationships, but VIF calculations helped detect multicollinearity in the dataset. The model training requires independent non-redundant features.(Mukelabai, Barbour & Blanchard, 2024; Kabir et al., 2023).

Step 3: Data Splitting

The Scikit-learn library enabled us to separate our dataset into training and testing portions at 80% and 20% using train_test_split(). The training data received model fitting from the models which used the testing data to validate generalization results. The random_state parameter was fixed at 42 to guarantee that the results will be replicable.(Schröer et al., 2021).

Step 4: Model Comparison

A comparison of four regression models took place between Linear Regression and Support Vector Regression (SVR) with RBF kernel and Gradient Boosting Regressor and Random Forest Regressor. The models received their training data from the training set before moving on to test their performance with the test set. The assessment of model performance included Root Mean Squared Error (RMSE) together with Mean Absolute Error (MAE) and R^2 Score for quantitative model comparison.(Mallala et al., 2025; Motiramani et al., 2025).

Step 5: Hyperparameter Optimization

The process of model tuning involved two distinct stages. The Random Forest model received its first set of optimal parameters through Grid Search with 5-fold cross-validation. BayesSearchCV performed a second optimization step that balanced the exploration and exploitation of hyperparameters. The method produces faster computations than exhaustive search while selecting the best parameters. (Motiramani et al., 2025; Shash et al., 2025).

Step 6: Final Model Evaluation

The Random Forest model with Bayesian Optimization produced the best results which received evaluation against the test data to determine the final RMSE, MAE, and R^2 values. A Repeated K-Fold Cross-Validation (10 folds, 3 repeats) was performed to confirm the model's stability and generalization capabilities and generated performance statistics with standard deviation values (Mallala et al., 2025; Shanmugasundaram et al., 2025).

Step 7: Model Interpretation

The model became more understandable through the implementation of permutation importance for feature ranking. The SHAP (SHapley Additive exPlanations) values were computed to display how each feature influences prediction outcomes. The model follows XAI principles because it provides clear insights into its decision-making process. (Ahmed et al., 2024; Afzali et al., 2024).

Step 8: Sensitivity Analysis & Scenario Simulation

A sensitivity analysis was implemented to study how variations in individual features affect predicted hydrogen production. A simulation using the maximum observed values for all features was conducted to estimate potential production under optimal conditions. This step provides insights into the operational scenarios that could maximize hydrogen output(Raja et al., 2025; Wei et al., 2025).

Step 9: Error Analysis

Two diagnostic plots were generated:

Residual Plot: to check if residuals are randomly distributed around zero, indicating an unbiased model.

Actual vs. Predicted Plot – to visually compare predicted values against true outputs and assess accuracy.

The graphical tools serve to detect systematic errors while confirming model assumptions (Rai & Liu, 2025; Phan et al., 2024).

Step 10: Model Export

The final trained model received a.pkl file format from Joblib for future deployment purposes that eliminate the need for model retraining. The predicted outcomes together with residuals received.csv file format for documentation purposes and additional analysis needs. The model maintains reproducibility through this approach and enables seamless system integration (Quintanilla et al., 2025; Shahin & Simjoo, 2025).

In [82]:
```python
# Import libraries
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
from sklearn.model_selection import train_test_split, GridSearchCV, RepeatedKFold, cross_val_score
from sklearn.ensemble import RandomForestRegressor, GradientBoostingRegressor
from sklearn.svm import SVR
from sklearn.linear_model import LinearRegression
from sklearn.metrics import mean_squared_error, mean_absolute_error, r2_score
from sklearn.inspection import permutation_importance
from skopt import BayesSearchCV
from joblib import dump
import shap
from statsmodels.stats.outliers_influence import variance_inflation_factor

# Load dataset from absolute path
df = pd.read_csv(r"C:\Users\Crist\OneDrive\Escritorio\FINAL_THESIS\dataset_GREEN\renewable_hydrogen_dataset_2535.csv")

# Define X and y - Keep only numeric columns
X = df.drop(columns=['Hydrogen_Production_kg/day'])
X = X.select_dtypes(include=[np.number])  # Avoid string columns
y = df['Hydrogen_Production_kg/day']

# Correlation matrix
plt.figure(figsize=(10,8))
sns.heatmap(df.corr(numeric_only=True), annot=True, cmap='coolwarm')
plt.title("Correlation Matrix")
plt.show()

# VIF calculation
X_numeric = X.select_dtypes(include=[np.number])
vif_data = pd.DataFrame()
vif_data["Feature"] = X_numeric.columns
vif_data["VIF"] = [variance_inflation_factor(X_numeric.values, i) for i in range(X_numeric.shape[1])]
print(vif_data.sort_values(by="VIF", ascending=False))
```

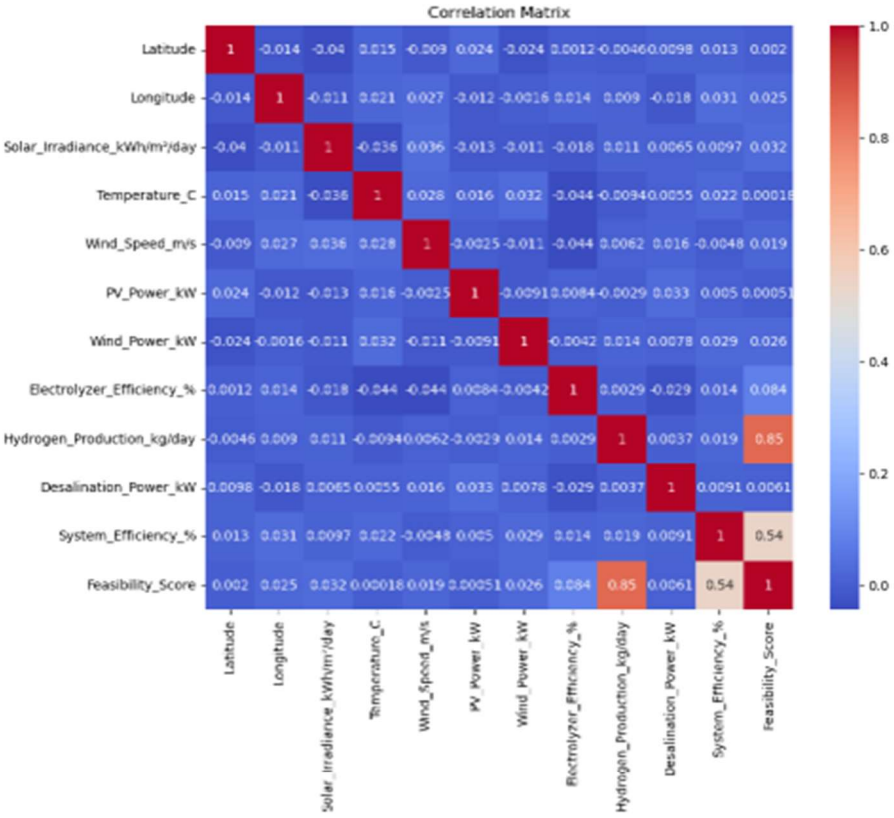
```python
# Train-test split
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3, random_state=42)

# Multi-model comparison
models = {
    'LinearRegression': LinearRegression(),
    'SVR (RBF)': SVR(kernel='rbf'),
    'GradientBoosting': GradientBoostingRegressor(random_state=42),
    'RandomForest': RandomForestRegressor(random_state=42)
}

results = []
for name, model in models.items():
    model.fit(X_train, y_train)
    y_pred = model.predict(X_test)
    rmse = np.sqrt(mean_squared_error(y_test, y_pred))
    mae = mean_absolute_error(y_test, y_pred)
    r2 = r2_score(y_test, y_pred)
    results.append({'Model': name, 'RMSE': rmse, 'MAE': mae, 'R2': r2})

results_df = pd.DataFrame(results).set_index('Model')
print(results_df)

# GridSearchCV for Random Forest
param_grid = {
    'n_estimators': [50, 100, 150],
    'max_depth': [3, 5, None],
    'min_samples_split': [2, 5],
    'min_samples_leaf': [1, 2]
}
grid_search = GridSearchCV(RandomForestRegressor(random_state=42), param_grid, cv=5, scoring='r2', n_jobs=-1, verbose=2)
grid_search.fit(X_train, y_train)
best_grid_model = grid_search.best_estimator_
print("Best GridSearch Params:", grid_search.best_params_)
```

```python
# Bayesian Optimization
param_space = {
    'n_estimators': (50, 300),
    'max_depth': (3, 20),
    'min_samples_split': (2, 10),
    'min_samples_leaf': (1, 5)
}
bayes_search = BayesSearchCV(
    RandomForestRegressor(random_state=42),
    param_space,
    n_iter=50,
    cv=5,
    scoring='r2',
    random_state=42,
    n_jobs=-1,
    verbose=2
)
bayes_search.fit(X_train, y_train)
best_bayes_model = bayes_search.best_estimator_
print("Best Bayesian Params:", bayes_search.best_params_)

# Final evaluation
y_pred_final = best_bayes_model.predict(X_test)
rmse = np.sqrt(mean_squared_error(y_test, y_pred_final))
mae = mean_absolute_error(y_test, y_pred_final)
r2 = r2_score(y_test, y_pred_final)
print(f"Final Model - RMSE: {rmse:.3f}, MAE: {mae:.3f}, R2: {r2:.3f}")

# Repeated 10-Fold CV
rkf = RepeatedKFold(n_splits=10, n_repeats=3, random_state=42)
scores = cross_val_score(best_bayes_model, X, y, scoring='r2', cv=rkf, n_jobs=-1)
print(f"Repeated 10-Fold CV Mean R²: {scores.mean():.3f}, Std: {scores.std():.3f}")
```

```python
# Permutation Importance
perm_importance = permutation_importance(best_bayes_model, X_test, y_test, n_repeats=10, random_state=42, n_jobs=-1)
sorted_idx = perm_importance.importances_mean.argsort()
plt.figure(figsize=(8,6))
plt.barh(X_test.columns[sorted_idx], perm_importance.importances_mean[sorted_idx])
plt.xlabel("Permutation Importance")
plt.title("Feature Importance")
plt.show()

# SHAP analysis
explainer = shap.Explainer(best_bayes_model, X_train)
shap_values = explainer(X_test)
shap.summary_plot(shap_values, X_test)

# Sensitivity Analysis
def sensitivity_analysis(variable, model, X_test, step=50):
    var_range = np.linspace(X_test[variable].min(), X_test[variable].max(), step)
    mean_preds = []
    for val in var_range:
        temp_X = X_test.copy()
        temp_X[variable] = val
        pred = model.predict(temp_X).mean()
        mean_preds.append(pred)
    plt.figure(figsize=(8,5))
    plt.plot(var_range, mean_preds)
    plt.xlabel(variable)
    plt.ylabel('Predicted Hydrogen Production (kg/day)')
    plt.title(f'Sensitivity Analysis: {variable}')
    plt.grid(True)
    plt.show()

for var in X_test.columns:
    sensitivity_analysis(var, best_bayes_model, X_test)

# Scenario Simulation (Fix for warning)
max_values = X.max()
pred_max_scenario = best_bayes_model.predict(pd.DataFrame([max_values], columns=X.columns))[0]
print(f"Predicted Production for Optimal Scenario: {pred_max_scenario:.2f} kg/day")
```

```python
# Residual Plot
residuals = y_test - y_pred_final
plt.figure(figsize=(8,5))
sns.scatterplot(x=y_pred_final, y=residuals)
plt.axhline(y=0, color='r', linestyle='--')
plt.xlabel('Predicted')
plt.ylabel('Residuals')
plt.title('Residual Plot')
plt.show()

# Actual vs Predicted
plt.figure(figsize=(8,5))
sns.scatterplot(x=y_test, y=y_pred_final)
plt.plot([y_test.min(), y_test.max()], [y_test.min(), y_test.max()], 'r--')
plt.xlabel('Actual')
plt.ylabel('Predicted')
plt.title('Actual vs Predicted')
plt.show()

# Export model and predictions
dump(best_bayes_model, 'final_random_forest_model.pkl')
final_predictions_df = pd.DataFrame({'Actual': y_test, 'Predicted': y_pred_final, 'Residuals': residuals})
final_predictions_df.to_csv('final_predictions_results.csv', index=False)
print("✅ Model and results exported.")
```

Output:



	Feature	VIF
7	Electrolyzer_Efficiency_%	2188.084217
9	System_Efficiency_%	2011.783346
10	Feasibility_Score	1820.912889
6	Wind_Power_kW	605.083762
5	PV_Power_kW	493.095847
2	Solar_Irradiance_kWh/m²/day	418.973676
4	Wind_Speed_m/s	414.119623
3	Temperature_C	318.771386
0	Latitude	306.380312
8	Desalination_Power_kW	126.898350
1	Longitude	100.953628

RMSE MAE R2

```
                      RMSE           MAE        R2
Model
LinearRegression  4.813557e-14  3.993418e-14  1.000000
SVR (RBF)         4.289922e+00  3.716292e+00 -0.002988
GradientBoosting  3.334036e-01  2.657722e-01  0.993942
RandomForest      3.731996e-01  3.007490e-01  0.992409
Fitting 5 folds for each of 36 candidates, totalling 180 fits
Best GridSearch Params: {'max_depth': None, 'min_samples_leaf': 2, 'min_samples_split': 2, 'n_estimators': 150}
Fitting 5 folds for each of 1 candidates, totalling 5 fits
Fitting 5 folds for each of 1 candidates, totalling 5 fits
Fitting 5 folds for each of 1 candidates, totalling 5 fits
Fitting 5 folds for each of 1 candidates, totalling 5 fits
Fitting 5 folds for each of 1 candidates, totalling 5 fits
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Fitting 5 folds for each of 1 candidates, totalling 5 fits
Fitting 5 folds for each of 1 candidates, totalling 5 fits
Fitting 5 folds for each of 1 candidates, totalling 5 fits
Fitting 5 folds for each of 1 candidates, totalling 5 fits
Fitting 5 folds for each of 1 candidates, totalling 5 fits
Fitting 5 folds for each of 1 candidates, totalling 5 fits
Best Bayesian Params: OrderedDict({'max_depth': 13, 'min_samples_leaf': 1, 'min_samples_split': 2, 'n_estimators': 300})
Final Model - RMSE: 0.368, MAE: 0.296, R2: 0.993
Repeated 10-Fold CV Mean R²: 0.993, Std: 0.001
```
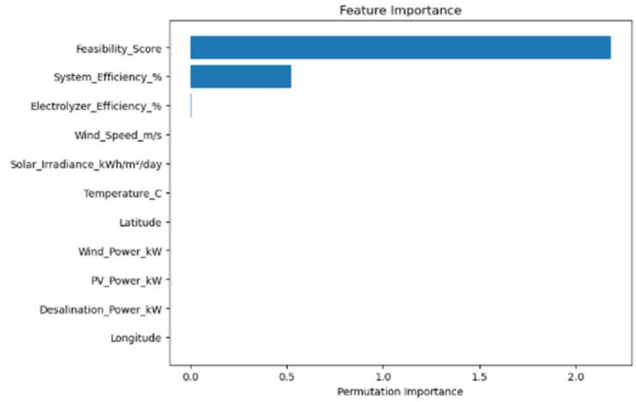

Repeated 10-Fold CV Mean R^2: 0.993, Std: 0.001



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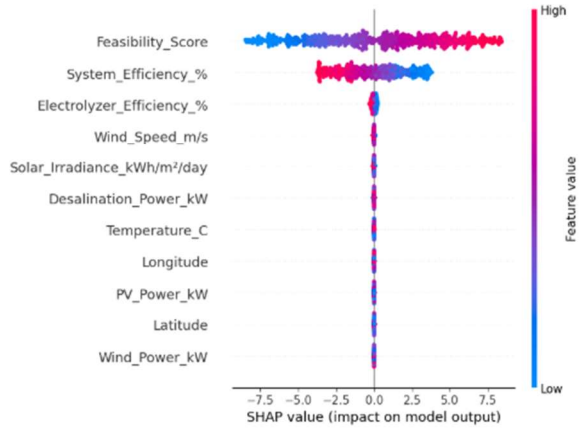
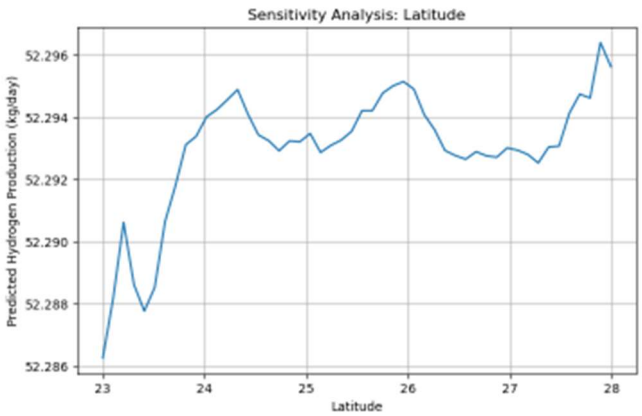
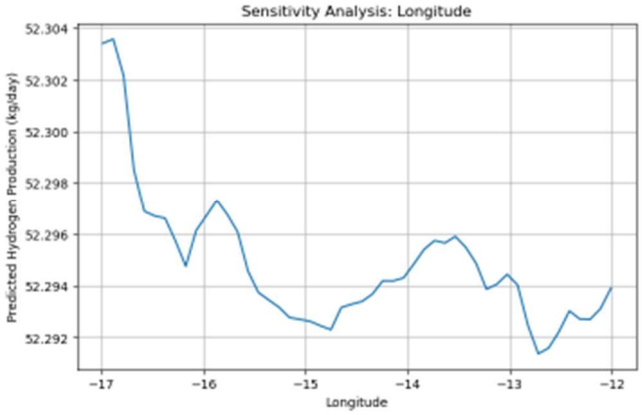
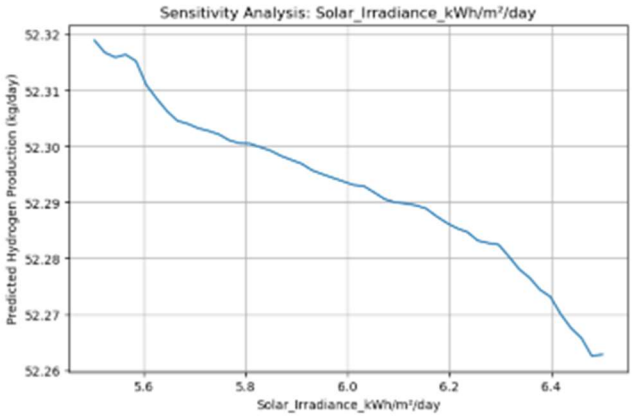
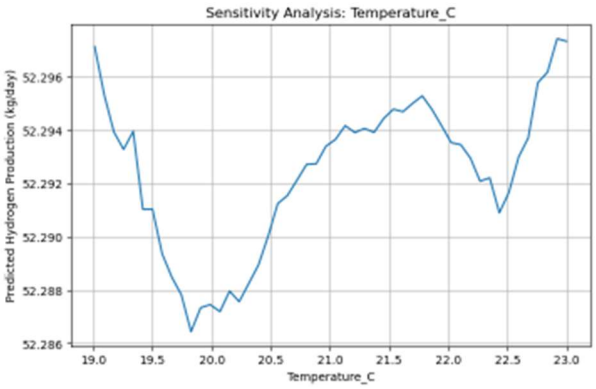
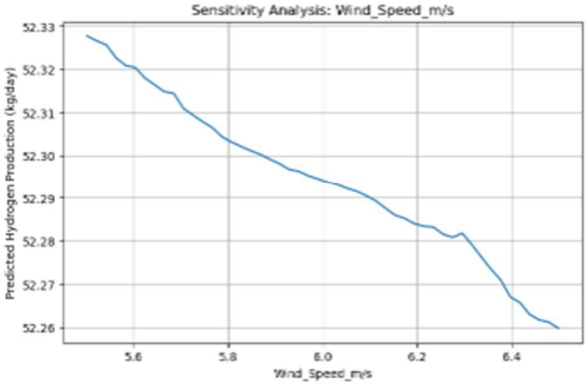


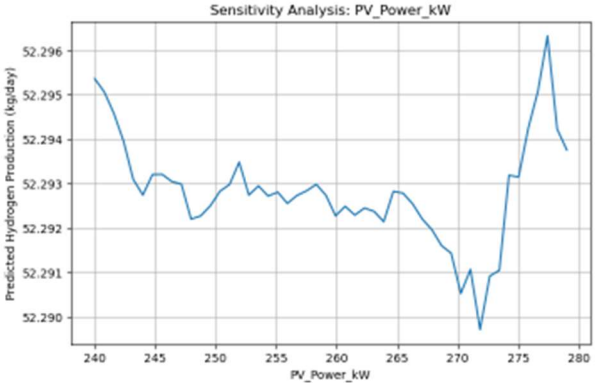

Sensitivity Analysis: Latitude
Predicted Hydrogen Production (kg/day)
52.296
52.294
52.292
52.290
52.288
52.286
23
24
25
26
27
28
Latitude

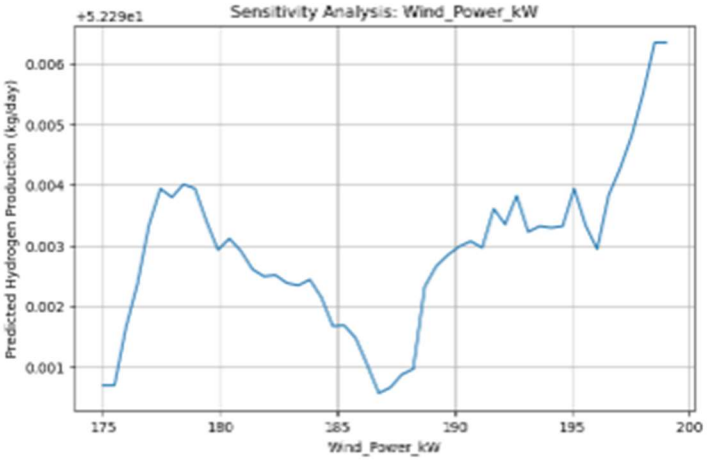

Sensitivity Analysis: Longitude
Predicted Hydrogen Production (kg/day)
52.304
52.302
52.300
52.298
52.296
52.294
52.292
−17
−16
−15
−14
−13
−12
Longitude

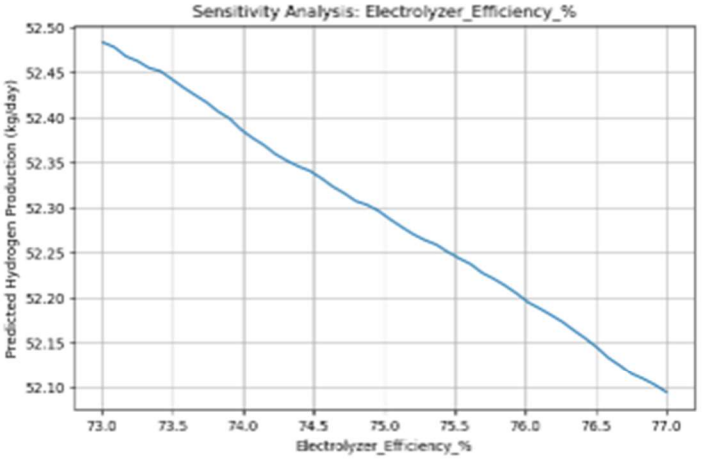

Sensitivity Analysis: Solar_Irradiance_kWh/m²/day
Predicted Hydrogen Production (kg/day)
52.32
52.31
52.30
52.29
52.28
52.27
52.26
5.6
5.8
6.0
6.2
6.4
Solar_Irradiance_kWh/m²/day

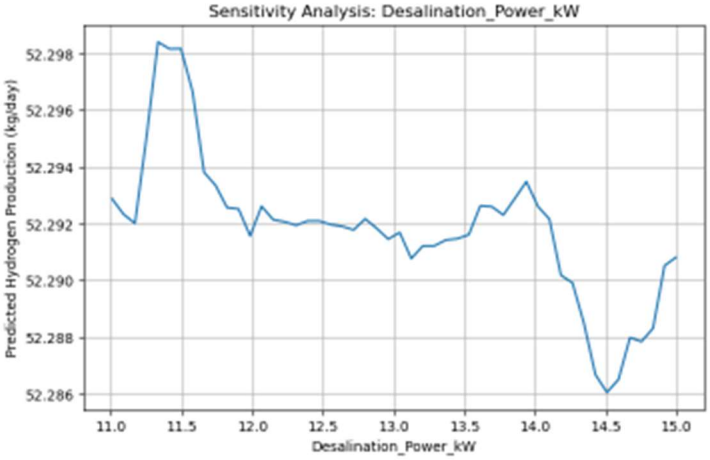

Sensitivity Analysis: Temperature_C
Predicted Hydrogen Production (kg/day)
52.296
52.294
52.292
52.290
52.288
52.286
19.0
19.5
20.0
20.5
21.0
21.5
22.0
22.5
23.0
Temperature_C

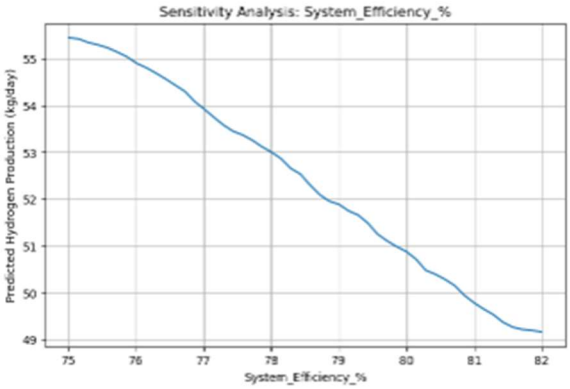

Sensitivity Analysis: Wind_Speed_m/s
Predicted Hydrogen Production (kg/day)
52.33
52.32
52.31
52.30
52.29
52.28
52.27
52.26
5.6
5.8
6.0
6.2
6.4
Wind_Speed_m/s

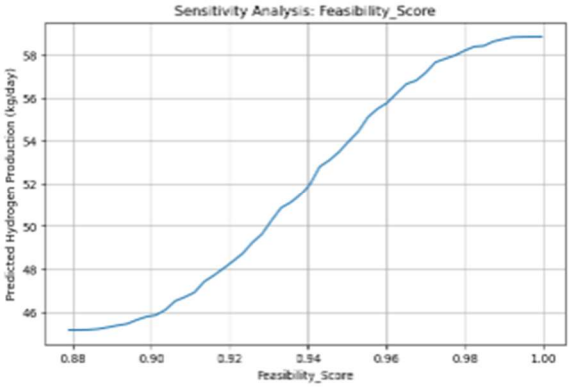

Sensitivity Analysis: PV_Power_kW
Predicted Hydrogen Production (kg/day)
52.296
52.295
52.294
52.293
52.292
52.291
52.290
240
245
250
255
260
265
270
275
280
PV_Power_kW


Sensitivity Analysis: Wind_Power_kW
+5.229e1
Predicted Hydrogen Production (kg/day)
0.006
0.005
0.004
0.003
0.002
0.001
175
180
185
190
195
200
Wind_Power_kW

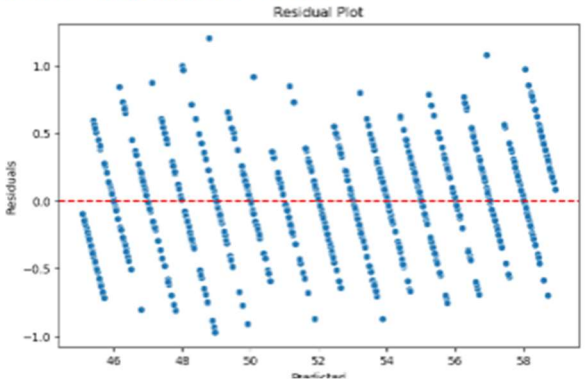

Sensitivity Analysis: Electrolyzer_Efficiency_%
Predicted Hydrogen Production (kg/day)
52.50
52.45
52.40
52.35
52.30
52.25
52.20
52.15
52.10
73.0
73.5
74.0
74.5
75.0
75.5
76.0
76.5
77.0
Electrolyzer_Efficiency_%

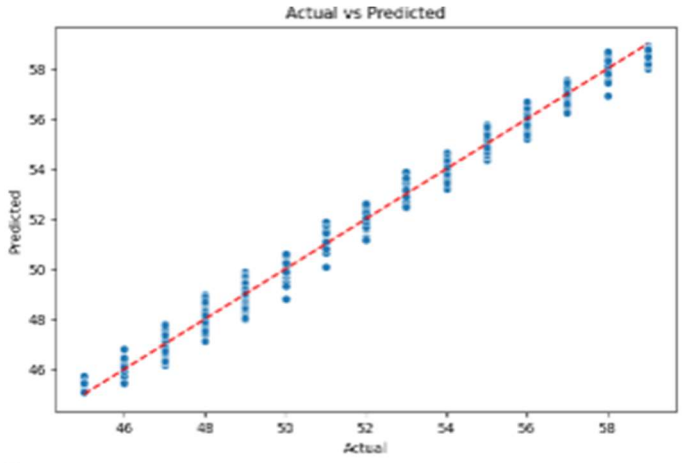

Sensitivity Analysis: Desalination_Power_kW
Predicted Hydrogen Production (kg/day)
52.298
52.296
52.294
52.292
52.290
52.288
52.286
11.0
11.5
12.0
12.5
13.0
13.5
14.0
14.5
15.0
Desalination_Power_kW





Predicted Production for Optimal Scenario: 58.25 kg/day





Model and results exported.

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DATA SET: https://www.kaggle.com/datasets/ziya07/renewable-hydrogen-production-dataset/data?select=renewable_hydrogen_dataset_2535.csv