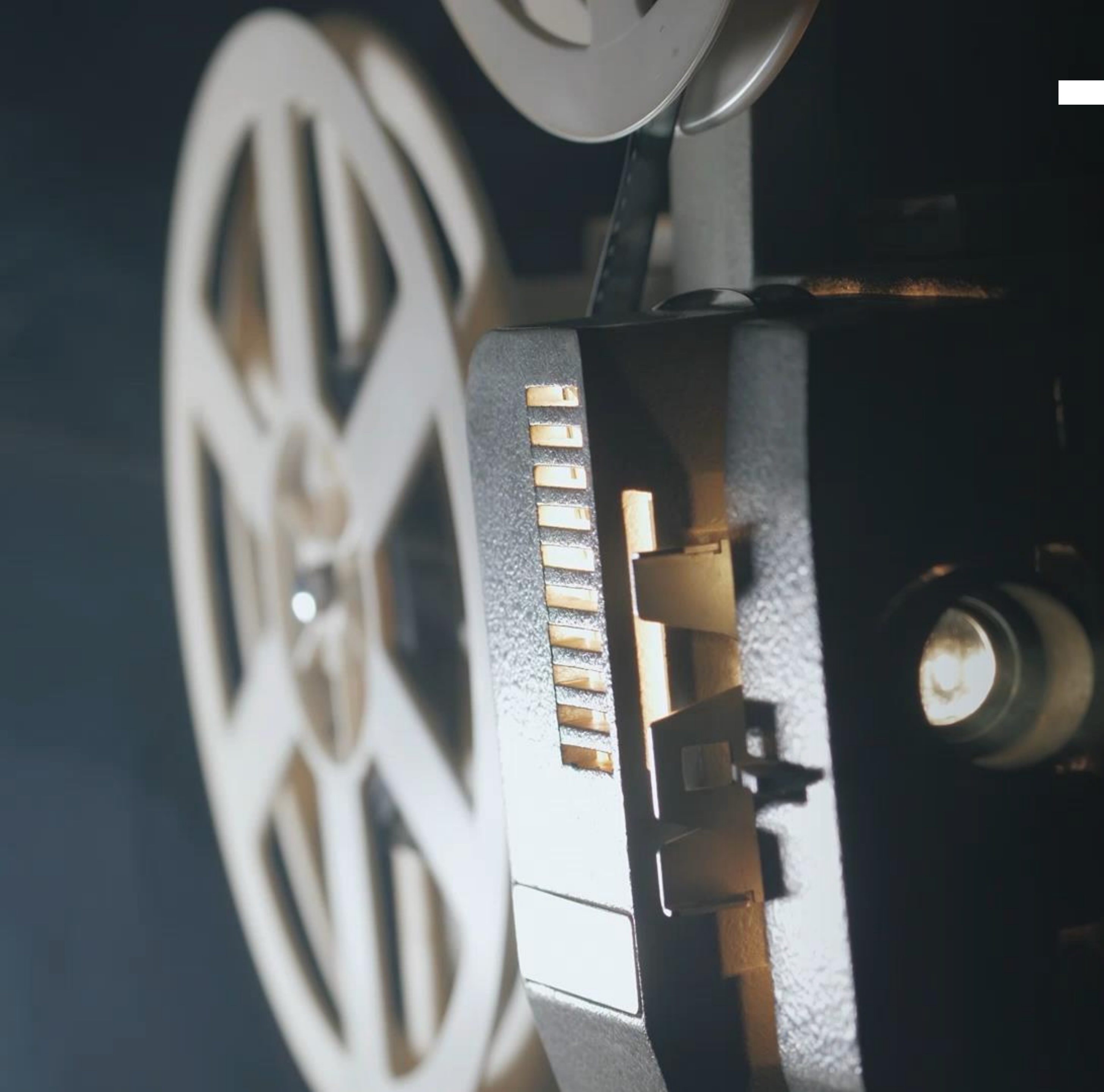


Machine Learning for Industrial Combustion System Optimization

Predicting NOx Emissions, CO2, and Temperature

Task 1: Data Cleaning (98.3% retention)

- Issues in data
  - Failed Thermocouples - Sensors showing impossible readings like 9999 C
  - Downtime periods - Times when the system was shutdown
  - Missing Values - Any NaN Values or Empty Values

```python
# get the shape of the raw dataframe
print('Before filtering:', df.shape)

# create a new dataframe using only rows where all thermocouples are valid
# the query removes data values greater than 5000 and also drops rows where the stoppage value is True
fildf = df.query('tc1 < 5000 and tc2 < 5000 and tc3 < 5000 \
    and tc4 < 5000 and tcf < 5000 \
    and stoppage == False').reset_index(drop=True)

print('After filtering:', fildf.shape)

# drop nan or empty values
print(fildf.isna().sum())
fildf = fildf.dropna()

# get the new dataframe shape
print('After filtering:', fildf.shape)
```

Results

Dataset:

- **4 Inputs:** Air flow, Air temperature, Oxygen fraction, Fuel flow
- **3 Outputs:** NOx emissions, Flue temperature, CO2 emissions

```
timestamp    0
air.flow     0
air.temp     0
air.frac     0
fuel.flow    0
tc1          0
tc2          0
tc3          0
tc4          0
tcf          0
f.h2o        0
f.co2        0
f.o2         0
f.ch4        0
f.nox        0
f.co         0
spec         0
stoppage     0
hub          0
shift        0
trial        0
dtype: int64
After filtering: (131699, 21)
```

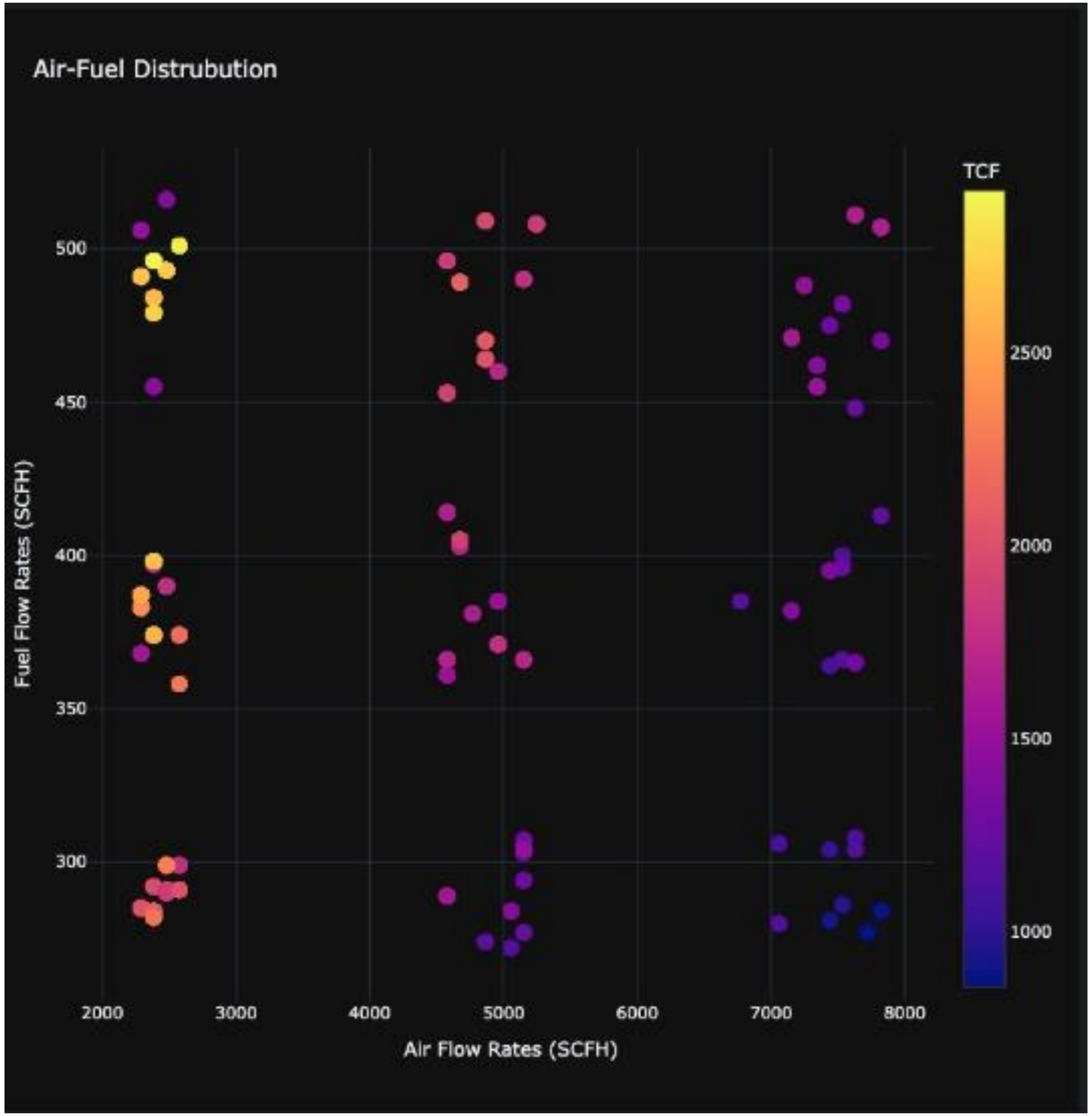
Checking for NaN or Empty values

After removing failed thermocouples and system stoppage

```
Before filtering: (133921, 21)
After filtering: (131699, 21)
```

Task 2 - Exploratory Analysis Key Findings

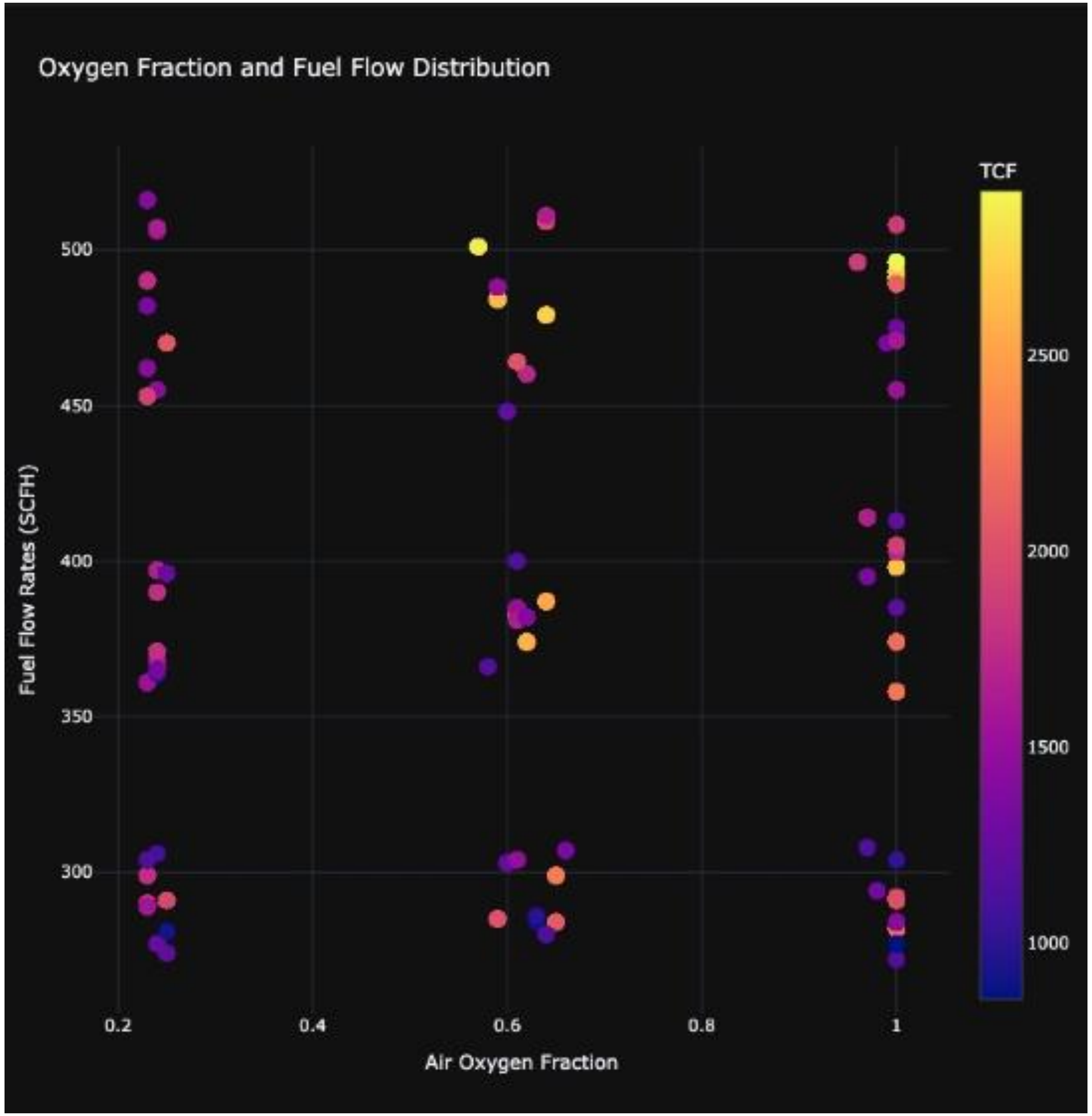
1. **Air-Fuel Ratio vs. Temperature**
   - **Low air flow** (2,500 SCFH) → High temp (2,000-2,700°C) - Yellow/Orange
   - **High air flow** (7,500 SCFH) → Low temp (1,000-1,500°C) - Blue/Purple
   - Air-fuel ratio is the dominant factor for temperature



EAKF - Continued

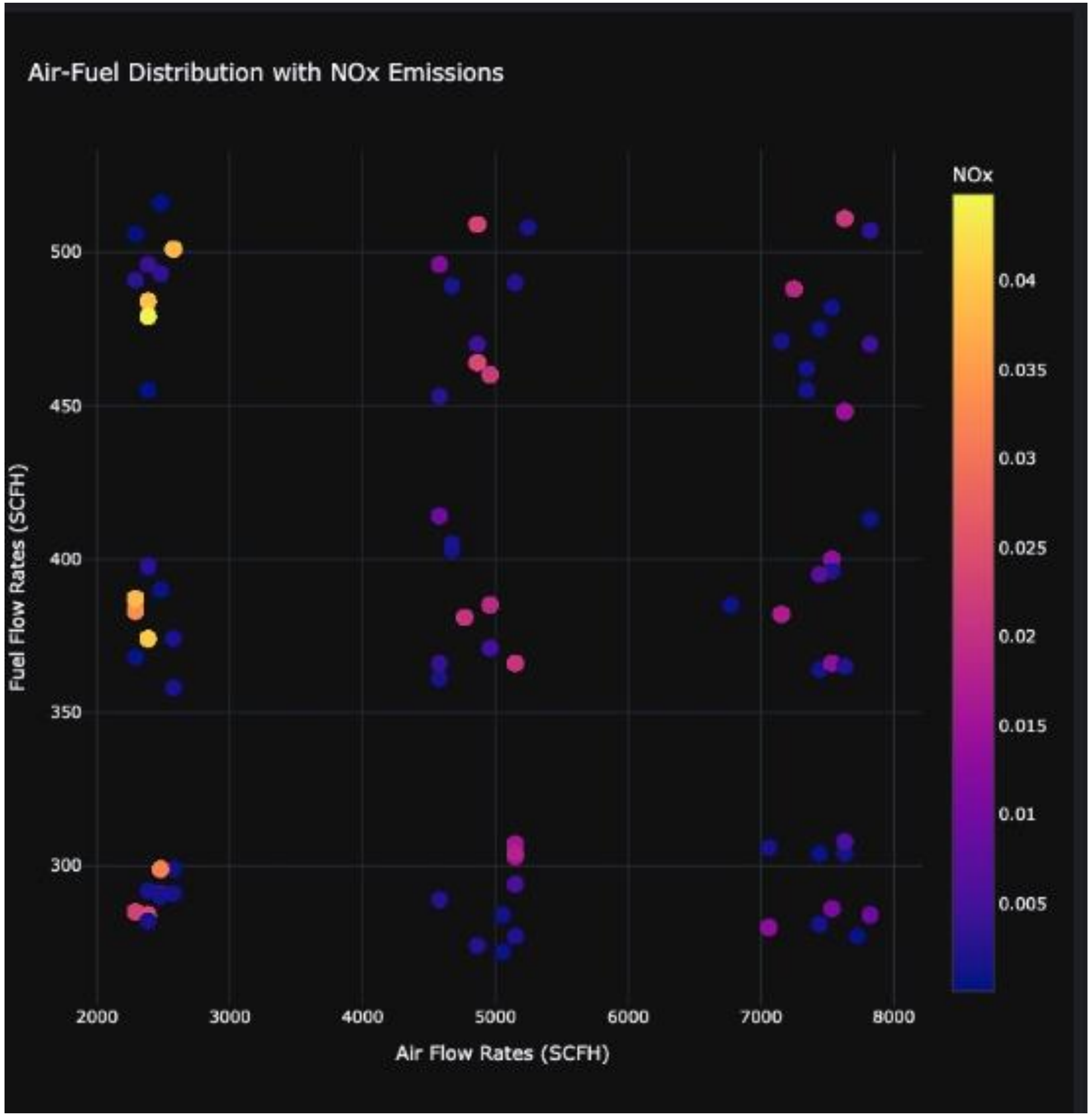
2. Oxygen Fraction vs. Temperature

- Pure oxygen (1.0) → 2,700°C (yellow)
- Normal air (0.21) → 1,200°C (blue)
- 1,000°C+ temperature increase from oxygen enrichment

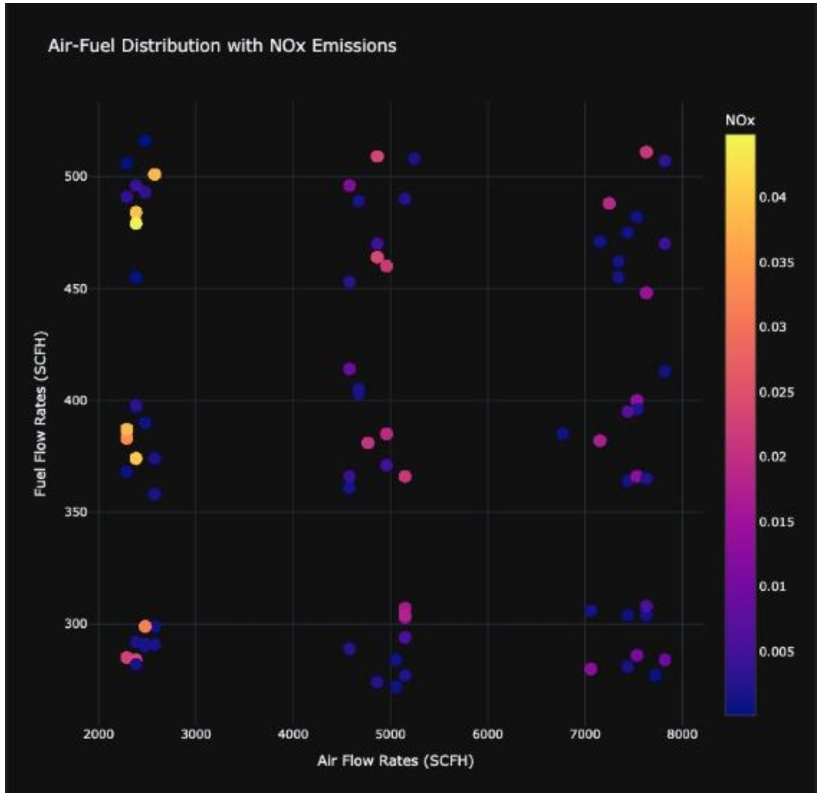


EAKF - Continued

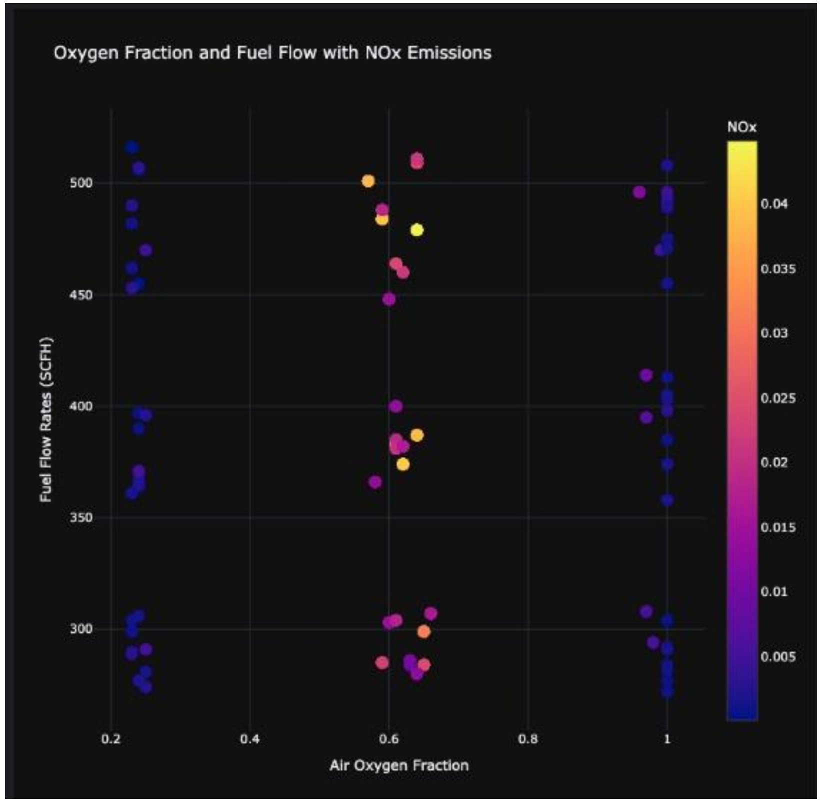
3. Air-Fuel Ratio vs. NOx Emission
   - Low air flow → High NOx (0.04-0.045) - Yellow
   - High air flow → Low NOx (0.002-0.01) - Blue
   - Direct correlation: High Temperature = High NOx



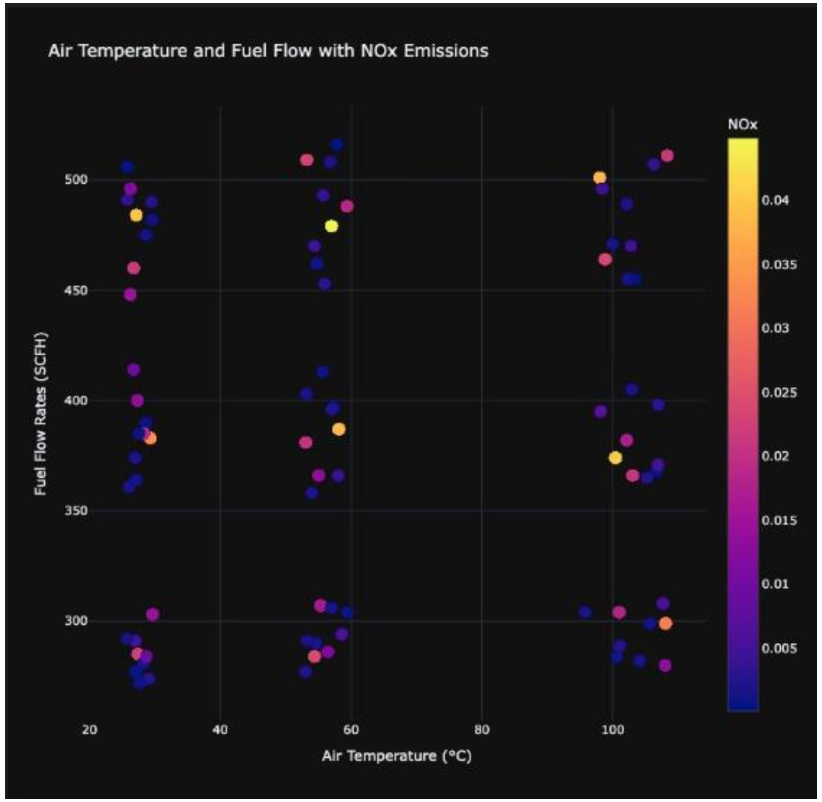
NOx Emissions Analysis (All Factors)



Air-Fuel vs NOx



Oxygen vs NOx



Air-Temp vs NOx

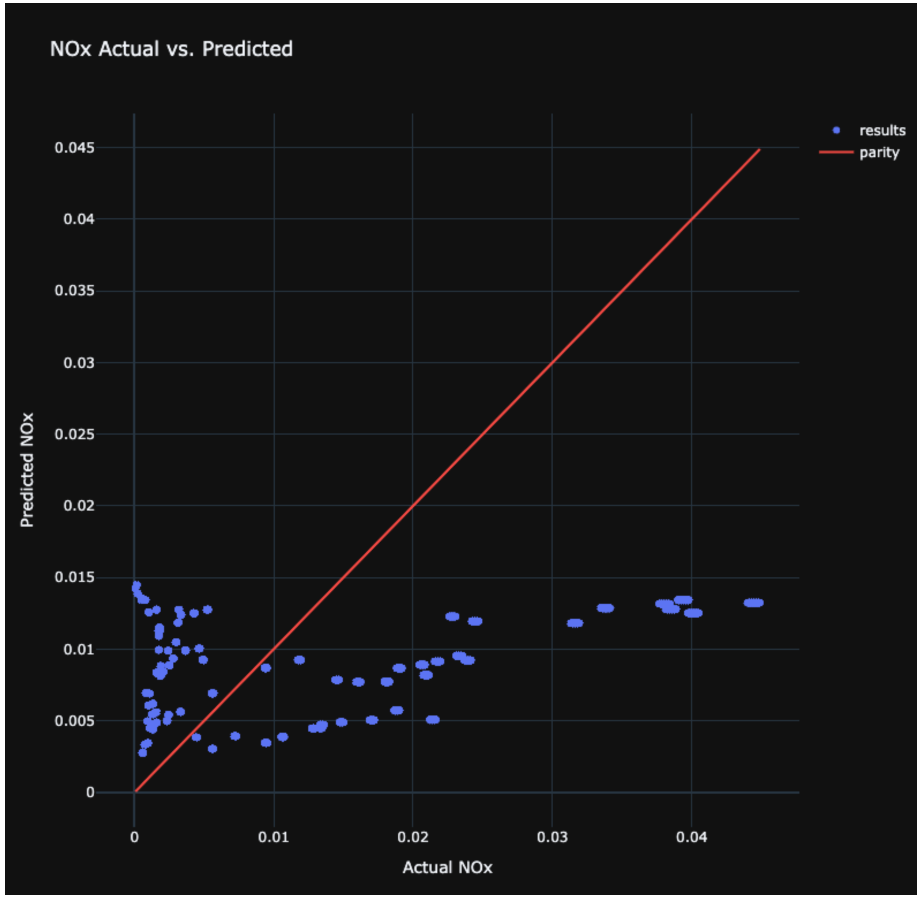
Task 3 - Linear Regression - Predict NOx

```
# Plot parity of actual versus predicted values
parity = go.Figure()

# add test v. predicted markers
parity.add_trace(
    go.Scatter(
        x=y_test['f.nox'],
        y=predictionsDF['f.nox'],
        mode='markers',
        name='results'
    )
)

# add parity line
parity.add_trace(
    go.Scatter(
        x=y_test['f.nox'],
        y=y_test['f.nox'],
        name='parity'
    )
)

# update layout and title
parity.update_layout(height=800, width=800, title="NOx Actual vs. Predicted")
parity.update_xaxes(title='Actual NOx')
parity.update_yaxes(title='Predicted NOx')
#display figure
parity.show()
```



'R2: 0.099349427556 1162'

Predict Flue temperature

```
# Build linear regression model for flue temperature (tcf)
# Use same train/test split as before
output_tcf = ['tcf']

# split the data into training (80%) and testing (20%) sets
X_train_tcf, X_test_tcf, y_train_tcf, y_test_tcf = train_test_split(
    df[inputs],
    df[output_tcf],
    test_size=0.2,
    random_state=42
)

# initiate the linear regression model
model_tcf = LinearRegression()

# fit the linear model using the input data
model_tcf.fit(X_train_tcf, y_train_tcf)

# determine r2 score for model
score_tcf = model_tcf.score(X_test_tcf, y_test_tcf)
display('R2 for TCF: ' + str(score_tcf))

# predict output for test data
predictions_tcf = model_tcf.predict(X_test_tcf)
predictionsDF_tcf = pd.DataFrame(predictions_tcf, columns=output_tcf)
```

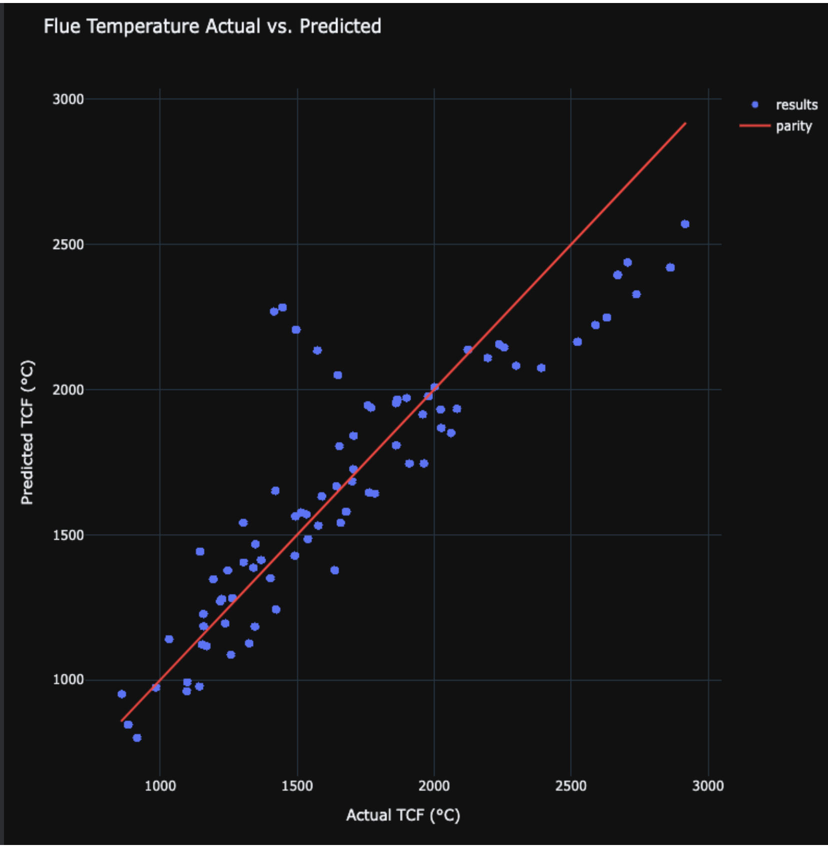
```
# Plot parity of actual versus predicted values for flue temperature
parity_tcf = go.Figure()

# add test v. predicted markers
parity_tcf.add_trace(
    go.Scatter(
        x=y_test_tcf['tcf'],
        y=predictionsDF_tcf['tcf'],
        mode='markers',
        name='results'
    )
)

# add parity line
parity_tcf.add_trace(
    go.Scatter(
        x=y_test_tcf['tcf'],
        y=y_test_tcf['tcf'],
        name='parity'
    )
)

# update layout and title
parity_tcf.update_layout(height=800, width=800, title="Flue Temperature Actual vs. Predicted")
parity_tcf.update_xaxes(title='Actual TCF (°C)')
parity_tcf.update_yaxes(title='Predicted TCF (°C)')

# display figure
parity_tcf.show()
```



'R2 for TCF: 0.7611991641990963'

Predict CO2 emissions

```python
# Build linear regression model for CO2 emissions (f.co2)
output_co2 = ['f.co2']

# split the data into training (80%) and testing (20%) sets
X_train_co2, X_test_co2, y_train_co2, y_test_co2 = train_test_split(
    df[inputs],
    df[output_co2],
    test_size=0.2,
    random_state=42
)

# initiate the linear regression model
model_co2 = LinearRegression()

# fit the linear model using the input data
model_co2.fit(X_train_co2, y_train_co2)

# determine r2 score for model
score_co2 = model_co2.score(X_test_co2, y_test_co2)
display('R2 for CO2: ' + str(score_co2))

# predict output for test data
predictions_co2 = model_co2.predict(X_test_co2)
predictionsDF_co2 = pd.DataFrame(predictions_co2, columns=output_co2)
```

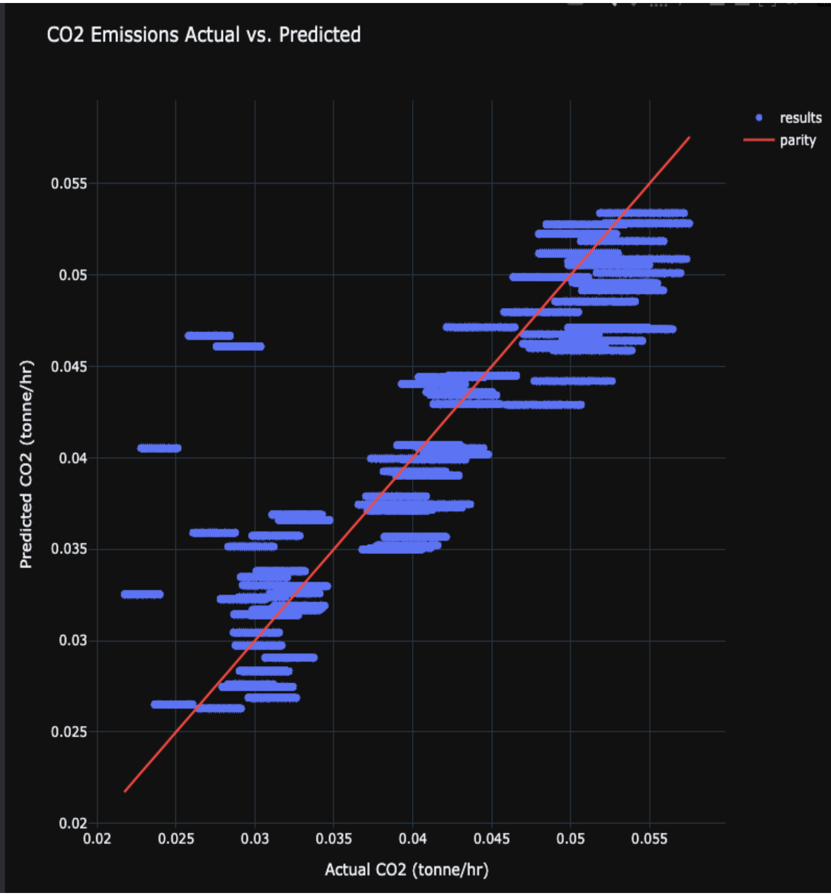
```python
# Plot parity of actual versus predicted values for CO2 emissions
parity_co2 = go.Figure()

# add test v. predicted markers
parity_co2.add_trace(
    go.Scatter(
        x=y_test_co2['f.co2'],
        y=predictionsDF_co2['f.co2'],
        mode='markers',
        name='results'
    )
)

# add parity line
parity_co2.add_trace(
    go.Scatter(
        x=y_test_co2['f.co2'],
        y=y_test_co2['f.co2'],
        name='parity'
    )
)

# update layout and title
parity_co2.update_layout(height=800, width=800, title="CO2 Emissions Actual vs. Predicted")
parity_co2.update_xaxes(title='Actual CO2 (tonne/hr)')
parity_co2.update_yaxes(title='Predicted CO2 (tonne/hr)')

# display figure
parity_co2.show()
```



'R2 for CO2: 0.7714021644644824'

Task 4 – LightGBM - NOx emissions

```python
# Build LightGBM model for NOx emissions
# Use the same train/test split as linear regression
# (you already have X_train, X_test, y_train, y_test for NOx)

# Create LightGBM regressor
model_lgb_nox = lgb.LGBMRegressor(
    n_estimators=100,
    learning_rate=0.1,
    random_state=42
)

# Fit the model using the training data
model_lgb_nox.fit(X_train, y_train)

# Predict on test data
predictions_lgb_nox = model_lgb_nox.predict(X_test)

# Create dataframe with predictions
predictionsDF_lgb_nox = pd.DataFrame(predictions_lgb_nox, columns=output)

# Calculate R² score
score_lgb_nox = model_lgb_nox.score(X_test, y_test)
display('LightGBM R2 for NOx: ' + str(score_lgb_nox))
```

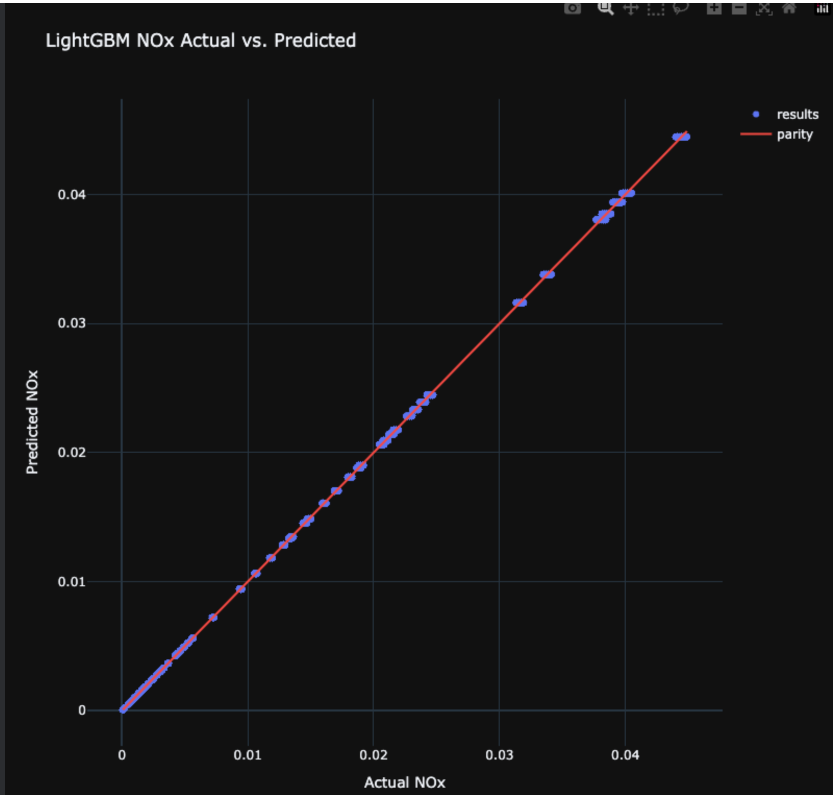
```python
# Plot parity of actual versus predicted values for LightGBM NOx model
parity_lgb_nox = go.Figure()

# add test v. predicted markers
parity_lgb_nox.add_trace(
    go.Scatter(
        x=y_test['f.nox'],
        y=predictionsDF_lgb_nox['f.nox'],
        mode='markers',
        name='results'
    )
)

# add parity line
parity_lgb_nox.add_trace(
    go.Scatter(
        x=y_test['f.nox'],
        y=y_test['f.nox'],
        name='parity'
    )
)

# update layout and title
parity_lgb_nox.update_layout(height=800, width=800, title="LightGBM NOx Actual vs. Predicted")
parity_lgb_nox.update_xaxes(title='Actual NOx')
parity_lgb_nox.update_yaxes(title='Predicted NOx')

# display figure
parity_lgb_nox.show()
```



'LightGBM R2 for NOx: 0.9999476812166448'

Predict Flue temperature

```python
# Build LightGBM model for flue temperature
# Use the same train/test split as linear regression for tcf

# Create LightGBM regressor
model_lgb_tcf = lgb.LGBMRegressor(
    n_estimators=100,
    learning_rate=0.1,
    random_state=42
)

# Fit the model using the training data
model_lgb_tcf.fit(X_train_tcf, y_train_tcf)

# Predict on test data
predictions_lgb_tcf = model_lgb_tcf.predict(X_test_tcf)

# Create dataframe with predictions
predictionsDF_lgb_tcf = pd.DataFrame(predictions_lgb_tcf, columns=output_tcf)

# Calculate R² score
score_lgb_tcf = model_lgb_tcf.score(X_test_tcf, y_test_tcf)
display('LightGBM R2 for TCF: ' + str(score_lgb_tcf))
```

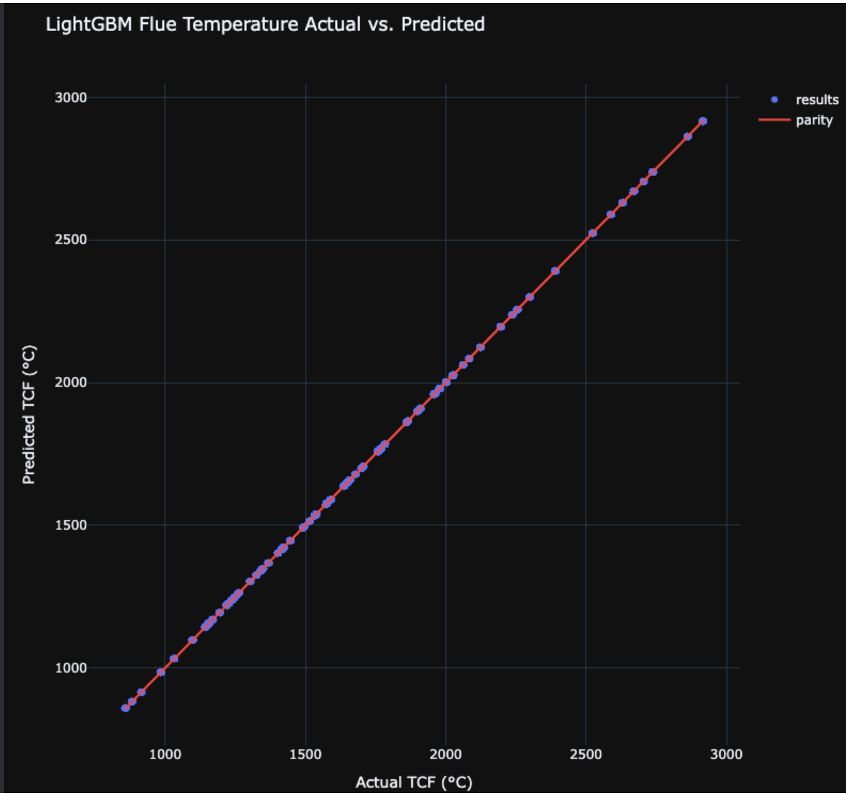
```python
# Plot parity of actual versus predicted values for LightGBM TCF model
parity_lgb_tcf = go.Figure()

# add test v. predicted markers
parity_lgb_tcf.add_trace(
    go.Scatter(
        x=y_test_tcf['tcf'],
        y=predictionsDF_lgb_tcf['tcf'],
        mode='markers',
        name='results'
    )
)

# add parity line
parity_lgb_tcf.add_trace(
    go.Scatter(
        x=y_test_tcf['tcf'],
        y=y_test_tcf['tcf'],
        name='parity'
    )
)

# update layout and title
parity_lgb_tcf.update_layout(height=800, width=800, title="LightGBM Flue Temperature Actual vs. Predicted")
parity_lgb_tcf.update_xaxes(title='Actual TCF (°C)')
parity_lgb_tcf.update_yaxes(title='Predicted TCF (°C)')

# display figure
parity_lgb_tcf.show()
```



'LightGBM R2 for TCF: 0.9999863375702582'

Predict CO2 Emissions

```python
 # Build LightGBM model for CO2 emissions
# Use the same train/test split as linear regression for CO2

# Create LightGBM regressor
model_lgb_co2 = lgb.LGBMRegressor(
    n_estimators=100,
    learning_rate=0.1,
    random_state=42
)

# Fit the model using the training data
model_lgb_co2.fit(X_train_co2, y_train_co2)

# Predict on test data
predictions_lgb_co2 = model_lgb_co2.predict(X_test_co2)

# Create dataframe with predictions
predictionsDF_lgb_co2 = pd.DataFrame(predictions_lgb_co2, columns=output_co2)

# Calculate R² score
score_lgb_co2 = model_lgb_co2.score(X_test_co2, y_test_co2)
display('LightGBM R2 for CO2: ' + str(score_lgb_co2))
```

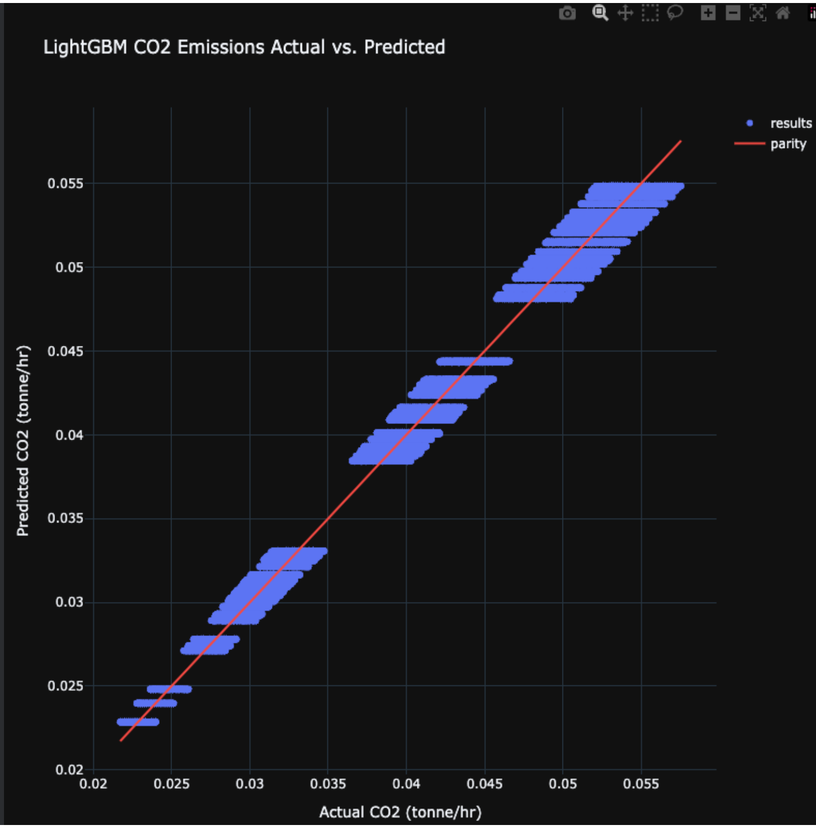
```python
# Plot parity of actual versus predicted values for LightGBM CO2 model
parity_lgb_co2 = go.Figure()

# add test v. predicted markers
parity_lgb_co2.add_trace(
    go.Scatter(
        x=y_test_co2['f.co2'],
        y=predictionsDF_lgb_co2['f.co2'],
        mode='markers',
        name='results'
    )
)

# add parity line
parity_lgb_co2.add_trace(
    go.Scatter(
        x=y_test_co2['f.co2'],
        y=y_test_co2['f.co2'],
        name='parity'
    )
)

# update layout and title
parity_lgb_co2.update_layout(height=800, width=800, title="LightGBM CO2 Emissions Actual vs. Predicted")
parity_lgb_co2.update_xaxes(title='Actual CO2 (tonne/hr)')
parity_lgb_co2.update_yaxes(title='Predicted CO2 (tonne/hr)')

# display figure
parity_lgb_co2.show()
```



'LightGBM R2 for CO2: 0.9833328919378389'

MAE Calculation

```
# Linear Regression MAE for NOx
mae_linear_nox = mean_absolute_error(y_test['f.nox'], predictionsDF['f.nox'])
display('Linear Regression MAE for NOx: ' + str(mae_linear_nox))

# LightGBM MAE for NOx
mae_lgb_nox = mean_absolute_error(y_test['f.nox'], predictionsDF_lgb_nox['f.nox'])
display('LightGBM MAE for NOx: ' + str(mae_lgb_nox))

# Comparison
display('NOx MAE Improvement: ' + str((mae_linear_nox - mae_lgb_nox) / mae_linear_nox * 100) + '%')
```

```
'Linear Regression MAE for NOx: 0.008213651320126048'
'LightGBM MAE for NOx: 4.059477595657994e-05'
'NOx MAE Improvement: 99.50576455738862%'
```

```
# Linear Regression MAE for TCF
mae_linear_tcf = mean_absolute_error(y_test_tcf['tcf'], predictionsDF_tcf['tcf'])
display('Linear Regression MAE for TCF: ' + str(mae_linear_tcf))

# LightGBM MAE for TCF
mae_lgb_tcf = mean_absolute_error(y_test_tcf['tcf'], predictionsDF_lgb_tcf['tcf'])
display('LightGBM MAE for TCF: ' + str(mae_lgb_tcf))

# Comparison
display('TCF MAE Improvement: ' + str((mae_linear_tcf - mae_lgb_tcf) / mae_linear_tcf * 100) + '%')
```

```
'Linear Regression MAE for TCF: 150.15417403922802'
'LightGBM MAE for TCF: 1.4928804860367397'
'TCF MAE Improvement: 99.00576824081712%'
```

```
# Linear Regression MAE for CO2
mae_linear_co2 = mean_absolute_error(y_test_co2['f.co2'], predictionsDF_co2['f.co2'])
display('Linear Regression MAE for CO2: ' + str(mae_linear_co2))

# LightGBM MAE for CO2
mae_lgb_co2 = mean_absolute_error(y_test_co2['f.co2'], predictionsDF_lgb_co2['f.co2'])
display('LightGBM MAE for CO2: ' + str(mae_lgb_co2))

# Comparison
display('CO2 MAE Improvement: ' + str((mae_linear_co2 - mae_lgb_co2) / mae_linear_co2 * 100) + '%')
```

```
'Linear Regression MAE for CO2: 0.0030279606345131075'
'LightGBM MAE for CO2: 0.0010353649994085008'
'CO2 MAE Improvement: 65.80652378345776%'
```

R2 & MAE Comparison

Performance Comparison

Model	Linear R2	LightGBM R2	Improvement
NOx	0.099	0.999	Yes
Temperature	0.761	0.999	Yes
CO2	0.771	0.983	Yes

Mean Absolute Error

Model	Linear MAE	LightGBM MAE	Reduction
NOx	0.00821	0.0000406	99.5%
Temperature	150.15	1.49	99.0%
CO2	0.00303	0.00104	65.8%