IMPORT NECESSARY LIBRARY

In [1]:
```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns

import warnings
warnings.simplefilter("ignore")
```

ADJUSTS THE DEFAULT FIGURE SIZE FOR MATPLOTLIB PLOTS

In [2]:
```
import matplotlib
matplotlib.rcParams['figure.figsize']=(12,6)
```

READ DATASET

In [3]:
```
#Load the data
fiber_data=pd.read_excel("E:/Intern/fiber_data.xlsx")
#fiber_data=fiber_data.drop(["Source","Solution (Solvent Ratio)"],axis=1)
```

DISPLAY THE FIRST AND LAST FIVE ROWS OF THE DATA

In [4]:
```
fiber_data
```

Out[4]:

	Source	Solvent	Solution (Solvent Ratio)	δ* =Sum of Products of Volume Fraction and δ of Individual Solvents	Ra* (HSP distance between Polymer & Solvent mixture)	Polymer Concentration (wt%)	RED	Voltage (kV)	Dist
0	K.P. Matabola, R.M. Moutloali, The influence o...	DMAC	1:0	22.771254	0.72111	22.0	0.075116	12	
1	NaN	DMAC	1:0	22.771254	0.72111	24.0	0.075116	12	
2	NaN	DMAC	1:0	22.771254	0.72111	26.0	0.075116	12	
3	NaN	DMAC	1:0	22.771254	0.72111	28.0	0.075116	12	
4	NaN	DMAC	1:0	22.771254	0.72111	28.0	0.075116	12	
...	...	...	...	...	...	...	...	...	
287	NaN	DMF	1:0	24.862421	2.10000	18.0	0.218700	11.3	
288	NaN	DMF	1:0	24.862421	2.10000	18.0	0.218700	11.8	
289	NaN	DMF	1:0	24.862421	2.10000	18.0	0.218700	12.3	
290	NaN	DMF	1:0	24.862421	2.10000	18.0	0.218700	12.8	
291	NaN	DMF	1:0	24.862421	2.10000	18.0	0.218700	13.5	

292 rows × 12 columns

DISPLAY COLUMNS NAME OF YOURS DATASET

In [5]:
```
fiber_data.columns
```

Out[5]:
```
Index(['Source', 'Solvent', 'Solution (Solvent Ratio)',
       'δ* =Sum of Products of Volume Fraction and δ of Individual Solvent
s',
       'Ra* (HSP distance between Polymer & Solvent mixture)',
       'Polymer Concentration (wt%)', 'RED ', 'Voltage (kV)', 'Distance (c
m)',
       'Feed (mL/h)', 'Flory-Huggins χ parameter', 'Fiber Diameter (nm)'],
      dtype='object')
```

DISPLAY THE SHAPE OF THE DATA

In [6]:
```
fiber_data.shape
```

Out[6]:
```
(292, 12)
```

SUMMARY OF THE DATA

In [7]:
```
fiber_data.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 292 entries, 0 to 291
Data columns (total 12 columns):
 #   Column
Non-Null Count  Dtype
---  ------
--------------  -----
 0   Source
31 non-null     object
 1   Solvent
292 non-null    object
 2   Solution (Solvent Ratio)
292 non-null    object
 3   δ* =Sum of Products of Volume Fraction and δ of Individual Solvents
292 non-null    float64
 4   Ra* (HSP distance between Polymer & Solvent mixture)
292 non-null    float64
 5   Polymer Concentration (wt%)
292 non-null    float64
 6   RED
292 non-null    float64
 7   Voltage (kV)
292 non-null    object
 8   Distance (cm)
292 non-null    object
 9   Feed (mL/h)
292 non-null    object
 10  Flory-Huggins χ parameter
292 non-null    float64
 11  Fiber Diameter (nm)
292 non-null    object
dtypes: float64(5), object(7)
memory usage: 27.5+ KB
```

CHANGE COLUMNS TYPE (OBJECT TO FLOAT)

In [8]:
```
for col in fiber_data.columns:
    if col in ["Voltage (kV)", "Distance (cm)", "Feed (mL/h)","Fiber Diamete
        fiber_data[col] = pd.to_numeric(fiber_data[col], errors='coerce')
```

FEATURE SELECTION (remove unwanted columns)

In [9]:
```
clear_fiber_data=fiber_data.iloc[:,5:]
```

In [10]:
```
clear_fiber_data
```

Out[10]:

	Polymer Concentration (wt%)	RED	Voltage (kV)	Distance (cm)	Feed (mL/h)	Flory-Huggins χ parameter	Fiber Diameter (nm)
0	22.0	0.075116	12.0	15.0	NaN	0.004855	98.0
1	24.0	0.075116	12.0	15.0	NaN	0.004855	155.0
2	26.0	0.075116	12.0	15.0	NaN	0.004855	240.0
3	28.0	0.075116	12.0	15.0	NaN	0.004855	397.0
4	28.0	0.075116	12.0	16.0	NaN	0.004855	314.0
...	...	...	...	...	...	...	...
287	18.0	0.218700	11.3	10.0	1.0	0.033900	203.1
288	18.0	0.218700	11.8	10.0	1.0	0.033900	148.2
289	18.0	0.218700	12.3	10.0	1.0	0.033900	203.0
290	18.0	0.218700	12.8	10.0	1.0	0.033900	194.2
291	18.0	0.218700	13.5	10.0	1.0	0.033900	153.0

292 rows × 7 columns

SUMMARY OF THE CLEAR_FIBER_DATA

In [11]:
```
clear_fiber_data.info()
```

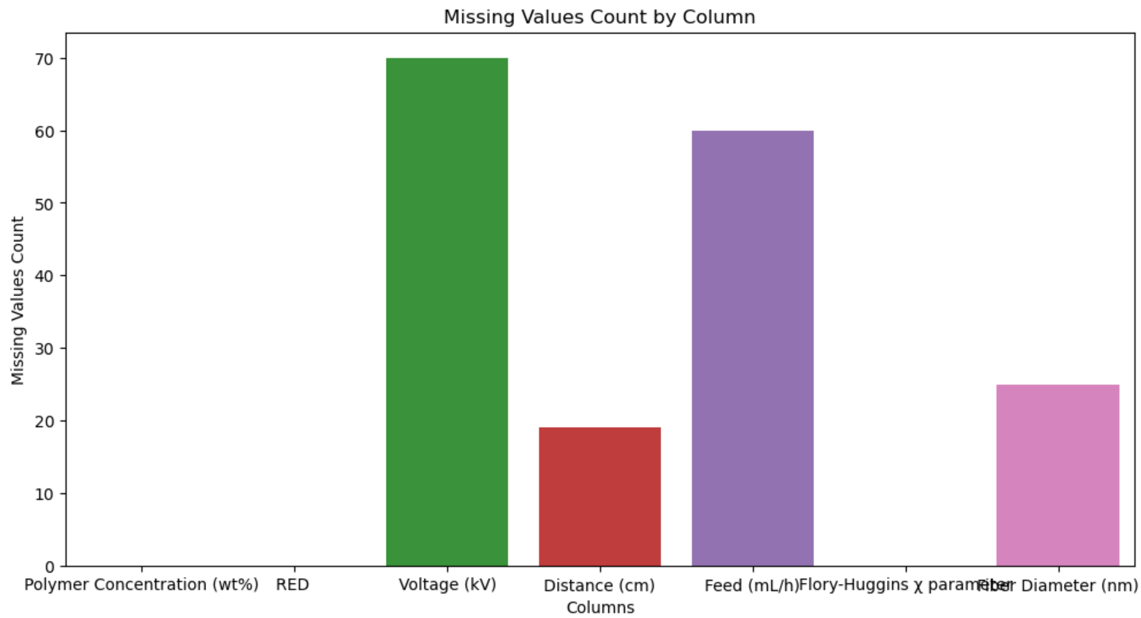
```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 292 entries, 0 to 291
Data columns (total 7 columns):
 #   Column                       Non-Null Count  Dtype  
---  ------                       --------------  -----  
 0   Polymer Concentration (wt%)  292 non-null    float64
 1   RED                          292 non-null    float64
 2   Voltage (kV)                 222 non-null    float64
 3   Distance (cm)                273 non-null    float64
 4   Feed (mL/h)                  232 non-null    float64
 5   Flory-Huggins χ parameter    292 non-null    float64
 6   Fiber Diameter (nm)          267 non-null    float64
dtypes: float64(7)
memory usage: 16.1 KB
```

TOTAL MISSING VALUES IN EACH COLUMNS

In [12]:
```
clear_fiber_data.isnull().sum()
```

Out[12]:
```
Polymer Concentration (wt%)     0
RED                             0
Voltage (kV)                   70
Distance (cm)                  19
Feed (mL/h)                    60
Flory-Huggins χ parameter       0
Fiber Diameter (nm)            25
dtype: int64
```

In [13]:
```
missing_values_count = clear_fiber_data.isnull().sum()

sns.barplot(x=missing_values_count.index, y=missing_values_count.values)
plt.xlabel('Columns')
plt.ylabel('Missing Values Count')
plt.title('Missing Values Count by Column')
plt.show()
```



DISPLAY NULL VALUE PERCENTAGE IN ASCENDING ORDER

In [14]:
```
missing_val=round((clear_fiber_data.isna().sum().sort_values()/len(clear_fib
missing_val
```

Out[14]:
```
Polymer Concentration (wt%)     0.0
RED                             0.0
Flory-Huggins χ parameter       0.0
Distance (cm)                   7.0
Fiber Diameter (nm)             9.0
Feed (mL/h)                    21.0
Voltage (kV)                   24.0
dtype: float64
```

In [15]:
```
missing_val=round(missing_val[missing_val>0])
```

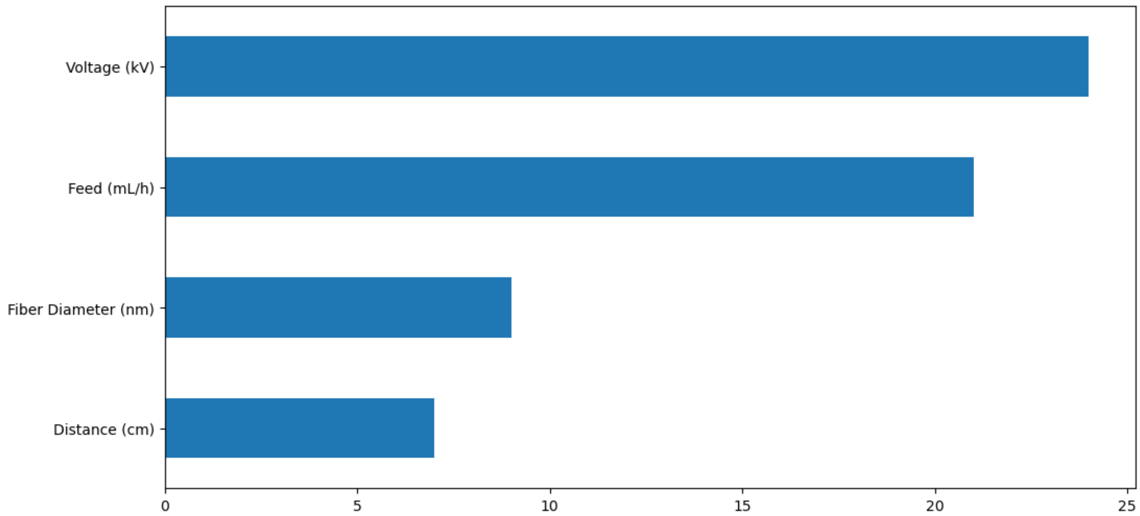
In [16]:
```
missing_val
```

Out[16]:
```
Distance (cm)          7.0
Fiber Diameter (nm)    9.0
Feed (mL/h)           21.0
Voltage (kV)          24.0
dtype: float64
```

VISUAL REPRESENTATION

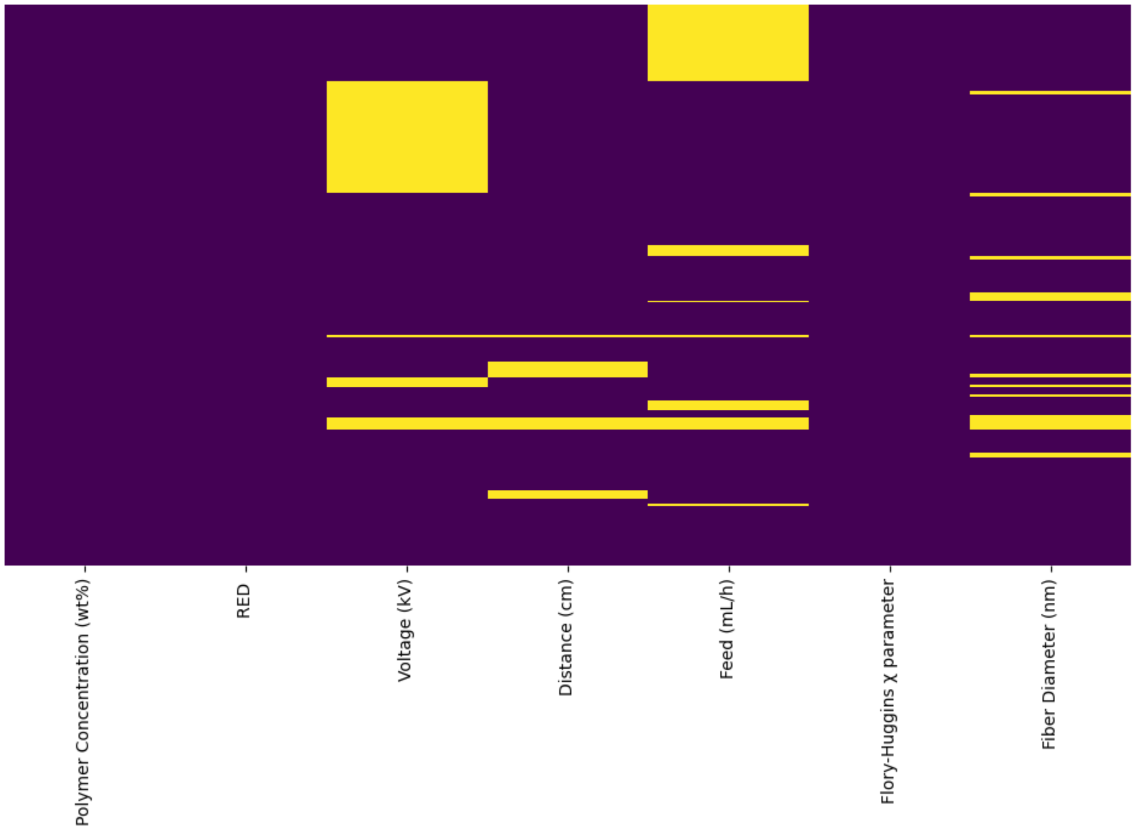
In [17]:
```
missing_val.plot(kind='barh')
```

Out[17]: <Axes: >



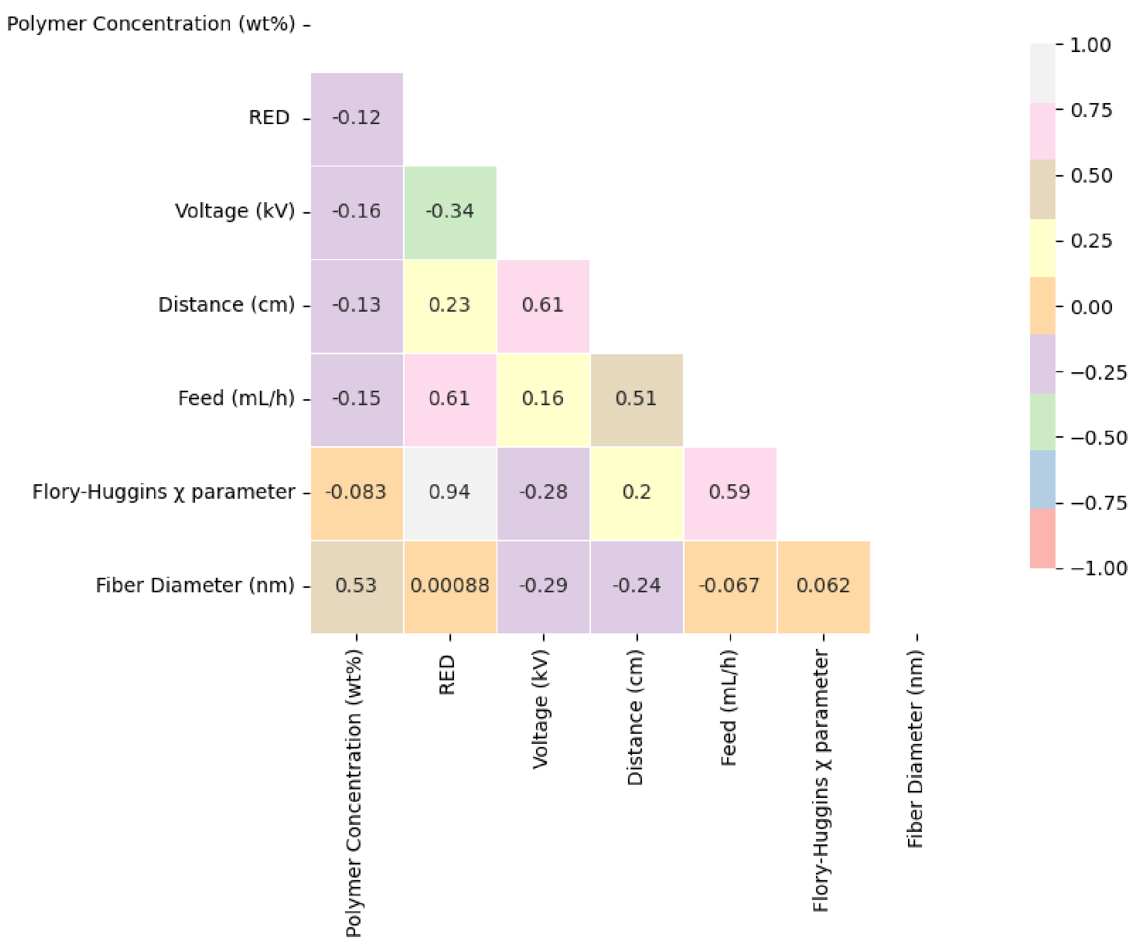
In [18]:
```
sns.heatmap(clear_fiber_data.isnull(),yticklabels=False,cbar=False,cmap='vir
```

Out[18]: <Axes: >



In [19]:
```
corr_matrix=clear_fiber_data.corr(method='spearman')

mask = np.zeros_like(corr_matrix, dtype=bool)
mask[np.triu_indices_from(mask)] = True

sns.heatmap(corr_matrix,yticklabels=True,cmap='Pastel1',
            mask=mask,annot=True, center=0, vmax=1, vmin =-1,
            square=True, linewidths=.5, cbar_kws={"shrink": .8})
```

Out[19]: <Axes: >

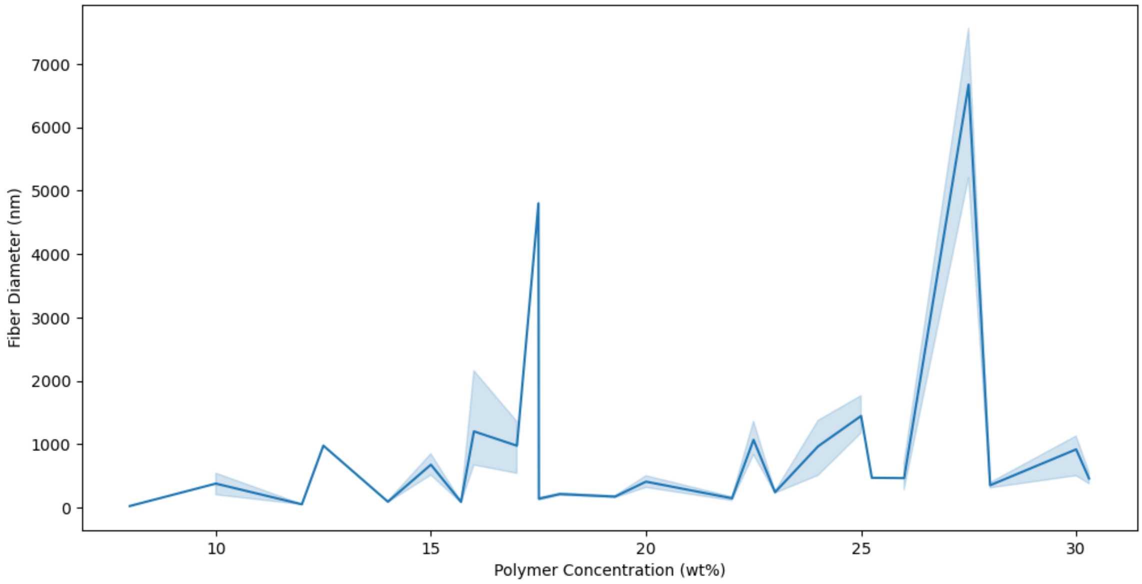


FILL THE MISSING VALUES

- Fiber Diameter (nm)

In [20]:
```
sns.lineplot(x='Polymer Concentration (wt%)',y='Fiber Diameter (nm)',data=fi
```

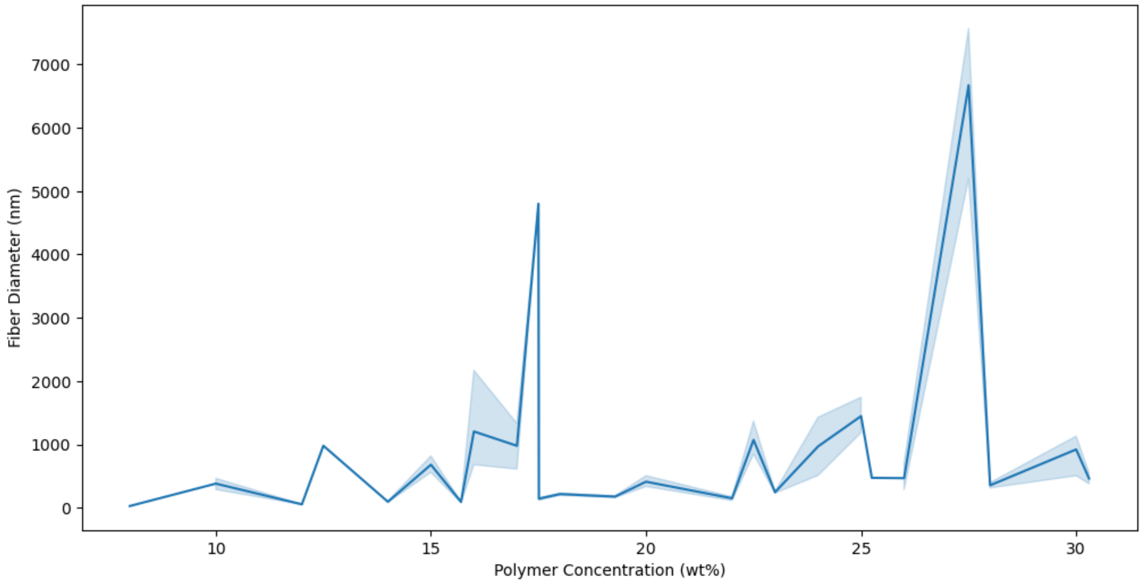
Out[20]: <Axes: xlabel='Polymer Concentration (wt%)', ylabel='Fiber Diameter (nm)'>



In [21]:
```
clear_fiber_data['Fiber Diameter (nm)'] = clear_fiber_data.groupby('Polymer
```

In [22]:
```
sns.lineplot(x='Polymer Concentration (wt%)',y='Fiber Diameter (nm)',data=cl
```

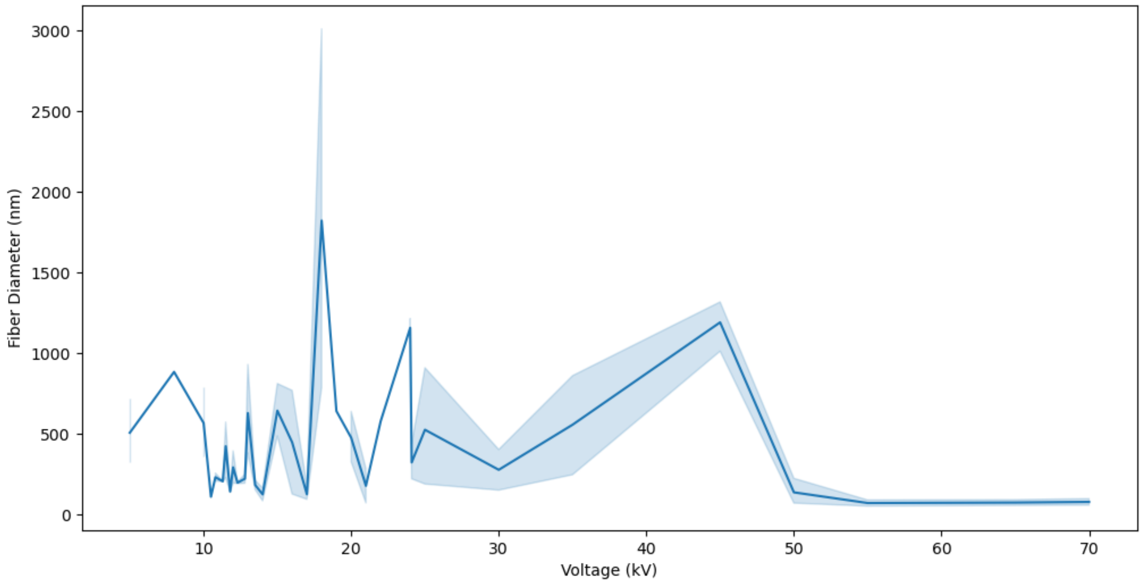
Out[22]: <Axes: xlabel='Polymer Concentration (wt%)', ylabel='Fiber Diameter (nm)'>



- 'Voltage (kV)'

In [23]:
```
sns.lineplot(x='Voltage (kV)',y='Fiber Diameter (nm)',data=fiber_data)
```

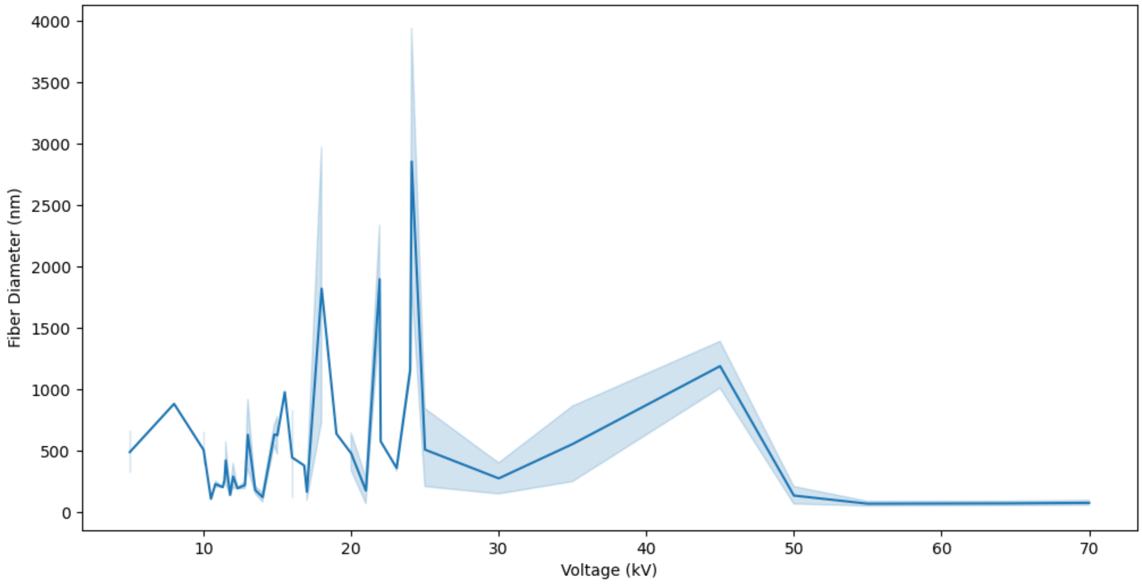
Out[23]: <Axes: xlabel='Voltage (kV)', ylabel='Fiber Diameter (nm)'>



In [24]:
```
clear_fiber_data['Voltage (kV)'] = clear_fiber_data.groupby('Polymer Concent
```

In [25]:
```
sns.lineplot(x='Voltage (kV)',y='Fiber Diameter (nm)',data=clear_fiber_data)
```

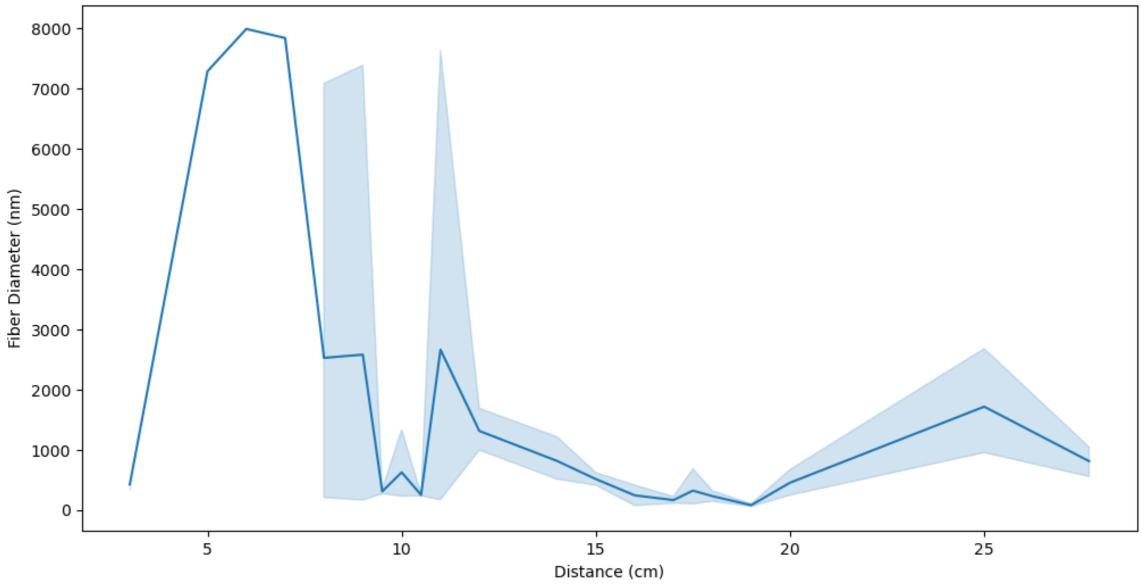
Out[25]: <Axes: xlabel='Voltage (kV)', ylabel='Fiber Diameter (nm)'>



- 'Distance (cm)'

In [26]:
```
sns.lineplot(x='Distance (cm)',y='Fiber Diameter (nm)',data=fiber_data)
```

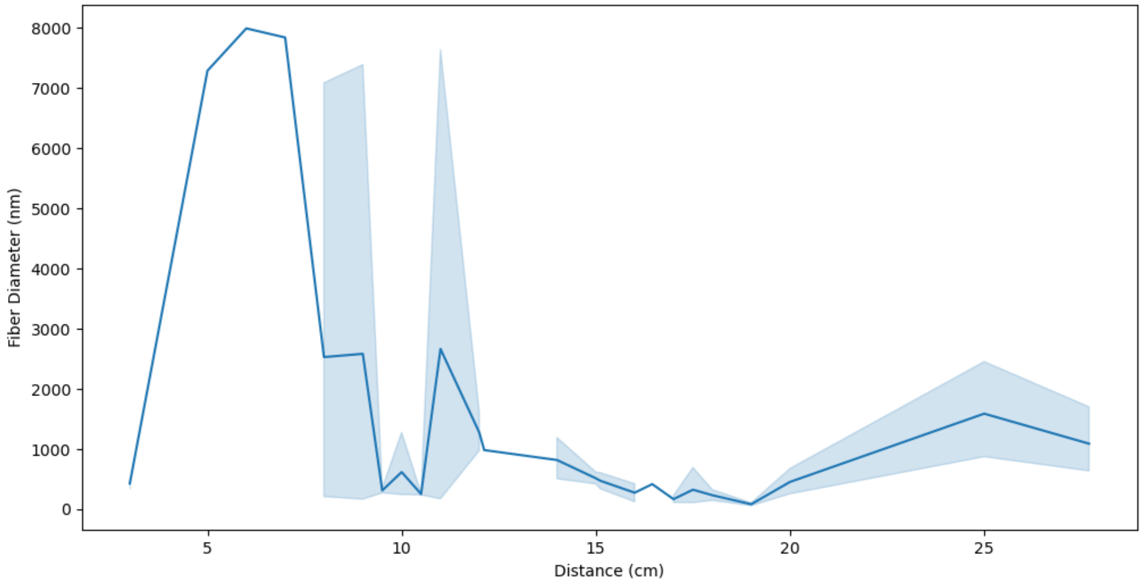
Out[26]: <Axes: xlabel='Distance (cm)', ylabel='Fiber Diameter (nm)'>



In [27]:
```
clear_fiber_data['Distance (cm)'] = clear_fiber_data.groupby('Polymer Concer
```

In [28]:
```
sns.lineplot(x='Distance (cm)',y='Fiber Diameter (nm)',data=clear_fiber_data
```

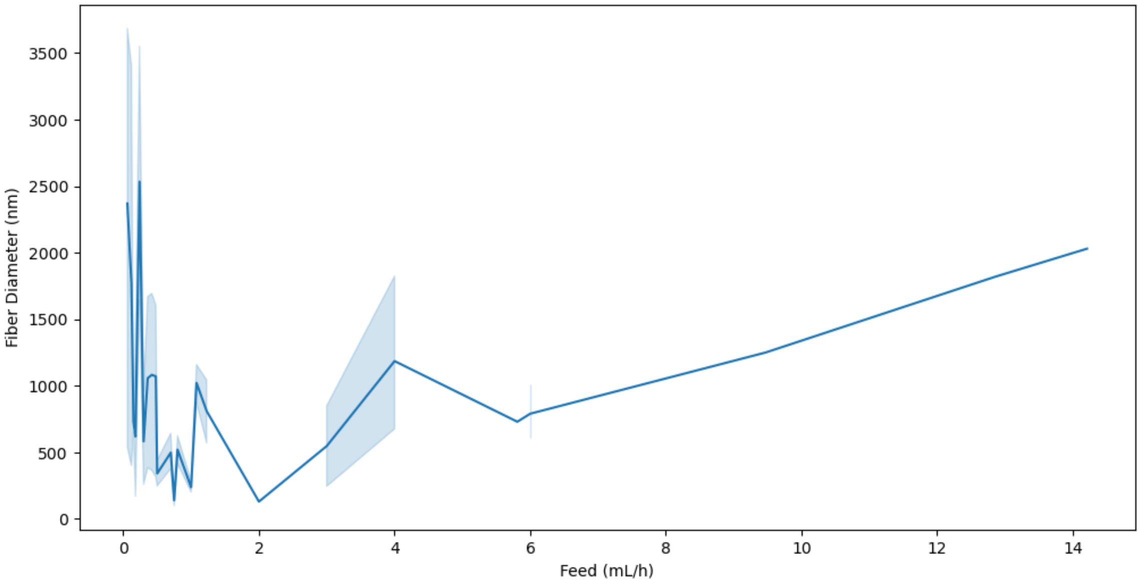
Out[28]: <Axes: xlabel='Distance (cm)', ylabel='Fiber Diameter (nm)'>



- FEED

In [29]:
```
sns.lineplot(x='Feed (mL/h)',y='Fiber Diameter (nm)',data=fiber_data)
```

Out[29]:
```
<Axes: xlabel='Feed (mL/h)', ylabel='Fiber Diameter (nm)'>
```



In [30]:
```
clear_fiber_data['Feed (mL/h)'] = clear_fiber_data.groupby('Polymer Concentr
```

In [31]:
```
clear_fiber_data.isnull().sum()
```

Out[31]:
```
Polymer Concentration (wt%)     0
RED                             0
Voltage (kV)                    1
Distance (cm)                   1
Feed (mL/h)                    23
Flory-Huggins χ parameter       0
Fiber Diameter (nm)             3
dtype: int64
```

In [32]:
```
missing_values_feed = clear_fiber_data[clear_fiber_data['Feed (mL/h)'].isnul
```

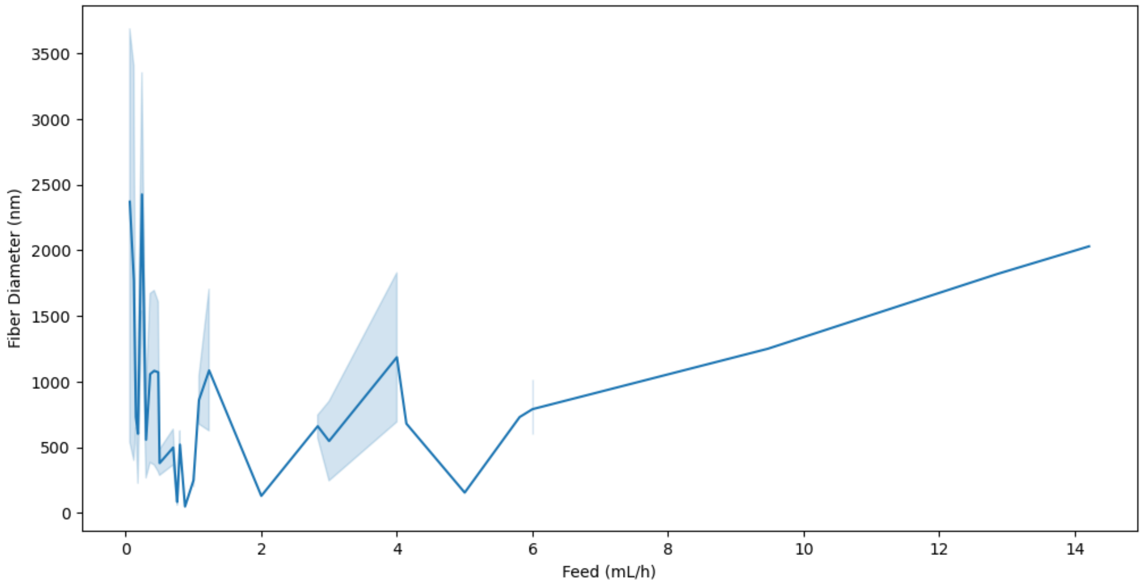
In [33]:
```
max_diameter=missing_values_feed['Fiber Diameter (nm)'].max()
```

In [34]:
```
#sns.lineplot(y='Feed (mL/h)',x='Fiber Diameter (nm)',data=clear_fiber_data[
```

In [35]:
```
clear_fiber_data.loc[clear_fiber_data['Fiber Diameter (nm)'] < max_diameter,
```

In [36]:
```
sns.lineplot(x='Feed (mL/h)',y='Fiber Diameter (nm)',data=clear_fiber_data)
```

Out[36]: <Axes: xlabel='Feed (mL/h)', ylabel='Fiber Diameter (nm)'>



In [37]:
```
clear_fiber_data.isnull().sum()
```

Out[37]:
```
Polymer Concentration (wt%)    0
RED                            0
Voltage (kV)                   1
Distance (cm)                  1
Feed (mL/h)                    2
Flory-Huggins χ parameter      0
Fiber Diameter (nm)            3
dtype: int64
```

DROP

In [38]:
```
clear_fiber_data=clear_fiber_data.dropna()
```

In [39]:
```
clear_fiber_data.describe()
```

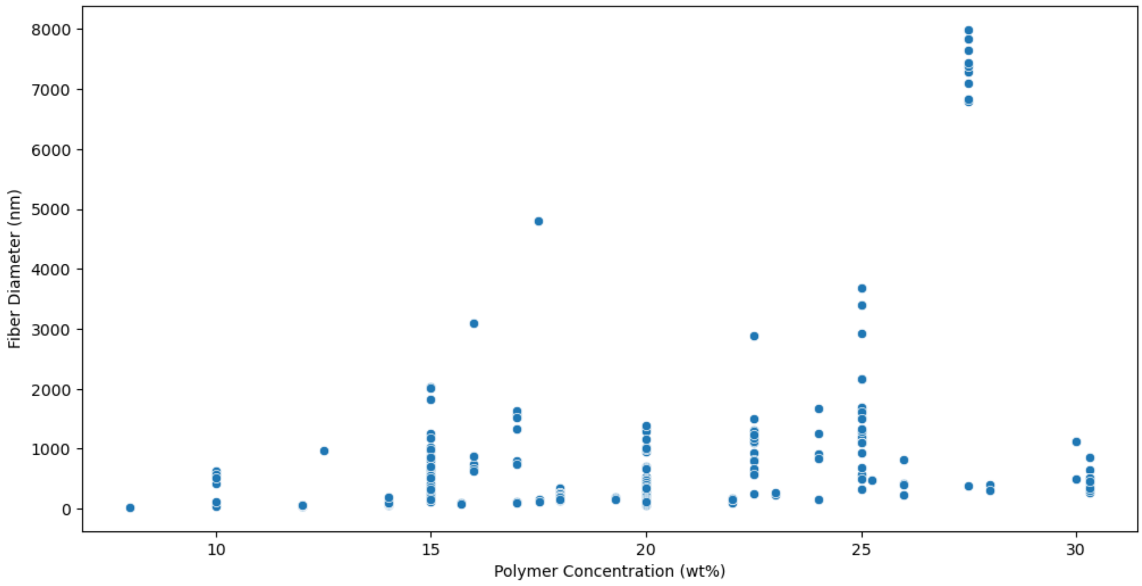
Out[39]:

	Polymer Concentration (wt%)	RED	Voltage (kV)	Distance (cm)	Feed (mL/h)	Flory-Huggins χ parameter	Fib Diamet (nn
count	288.000000	288.000000	288.000000	288.000000	288.000000	288.000000	288.00000
mean	19.212917	0.162954	22.368104	15.351013	1.207058	0.026135	818.70426
std	5.128778	0.096776	13.134601	4.633670	1.704752	0.028241	1360.10954
min	8.000000	0.075116	5.000000	3.000000	0.060000	0.004041	28.00000
25%	15.000000	0.075116	14.000000	12.000000	0.465000	0.004888	167.52500
50%	20.000000	0.103183	20.000000	15.000000	0.700000	0.007533	382.83333
75%	22.500000	0.218750	24.100000	18.000000	1.080000	0.034500	893.00000
max	30.300000	0.490026	70.000000	27.700000	14.210000	0.165076	7994.00000

VISUALIZATION

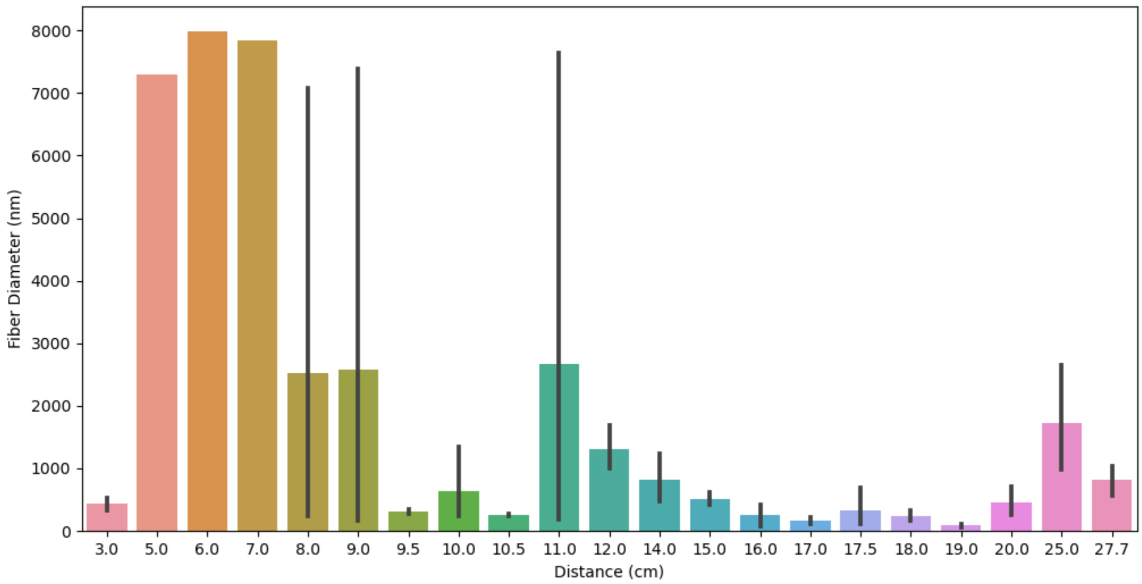
In [40]:
```
sns.scatterplot(data=fiber_data, x='Polymer Concentration (wt%)', y='Fiber D
```

Out[40]: <Axes: xlabel='Polymer Concentration (wt%)', ylabel='Fiber Diameter (nm)'>



In [41]:
```
sns.barplot(x='Distance (cm)',y='Fiber Diameter (nm)',data=fiber_data)
```

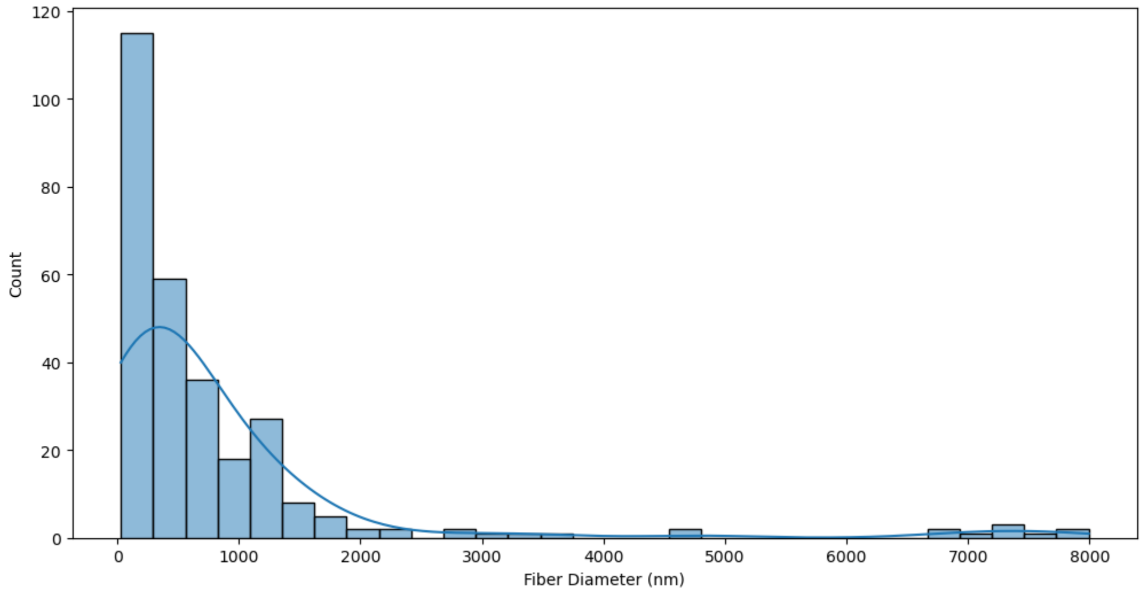
Out[41]: <Axes: xlabel='Distance (cm)', ylabel='Fiber Diameter (nm)'>



In [ ]:

In [42]:
```
sns.histplot(data=clear_fiber_data, x='Fiber Diameter (nm)', bins=30, kde=Tr
```

Out[42]: <Axes: xlabel='Fiber Diameter (nm)', ylabel='Count'>



MODEL BUILDING

In [43]:
```
X = clear_fiber_data.drop("Fiber Diameter (nm)",axis=1)
y = clear_fiber_data["Fiber Diameter (nm)"]
```

In [44]:
```
from sklearn.preprocessing import StandardScaler, MinMaxScaler


# Create an instance of the StandardScaler
scaler = StandardScaler()

# Define the columns you want to standardize
columns_to_standardize = ['Polymer Concentration (wt%)', 'Voltage (kV)', 'Di

# Apply standardization to the selected columns
#X[columns_to_standardize] = scaler.fit_transform(X[columns_to_standardize])

# Create an instance of the MinMaxScaler
minmax_scaler = MinMaxScaler(feature_range=(0, 1))

# Apply normalization to the selected columns
X[columns_to_standardize] = minmax_scaler.fit_transform(X[columns_to_standar
```

In [45]:
```
X.describe()
```

Out[45]:

	Polymer Concentration (wt%)	RED	Voltage (kV)	Distance (cm)	Feed (mL/h)	Flory-Huggins χ parameter
count	288.000000	288.000000	288.000000	288.000000	288.000000	288.000000
mean	0.502821	0.162954	0.267202	0.500041	0.081064	0.026135
std	0.229990	0.096776	0.202071	0.187598	0.120477	0.028241
min	0.000000	0.075116	0.000000	0.000000	0.000000	0.004041
25%	0.313901	0.075116	0.138462	0.364372	0.028622	0.004888
50%	0.538117	0.103183	0.230769	0.485830	0.045230	0.007533
75%	0.650224	0.218750	0.293846	0.607287	0.072085	0.034500
max	1.000000	0.490026	1.000000	1.000000	1.000000	0.165076

TRAIN_TEST_SPLIT

In [46]:
```
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size = 0.2, r
```

RandomForestRegressor

In [47]:
```
from sklearn.model_selection import GridSearchCV
from sklearn.ensemble import RandomForestRegressor

# Create the RandomForestRegressor model
model_1=RandomForestRegressor()

# Define the hyperparameters and their values to search over
model_1_param_grid = {

    'n_estimators': [3,5,10,20,50],
    'max_depth': [None, 5, 10],
    'min_samples_split': [2, 5, 10],
    'min_samples_leaf': [1, 2, 5, 10],
    'max_features': ['auto', 'sqrt', 'log2', None]

}

model_1_num_combination = 1

for model_1_k in model_1_param_grid.keys():
    model_1_num_combination *= len(model_1_param_grid[model_1_k])

print("Number of Combinations: ", model_1_num_combination)

# Perform grid search
model_1_grid_search = GridSearchCV(estimator=model_1, param_grid=model_1_par
model_1_grid_search.fit(X_train, y_train)
```

```
Number of Combinations:  720
```

Out[47]:
```
▸ GridSearchCV
▸ estimator: RandomForestRegressor
    ▸ RandomForestRegressor
```

In [48]:
```
# Get the best hyperparameters and the best model for model_1
model_1_best_params = model_1_grid_search.best_params_
model_1_best_model = model_1_grid_search.best_estimator_
```

In [49]:
```
model_1_best_params
```

Out[49]:
```
{'max_depth': 10,
 'max_features': 'log2',
 'min_samples_leaf': 2,
 'min_samples_split': 5,
 'n_estimators': 5}
```

In [50]:
```
from sklearn.metrics import mean_absolute_error, mean_squared_error, r2_scor

# Model_1 Train evaluation

y_predict_model_1_train = model_1_grid_search.predict(X_train)

model_1_mae_train = mean_absolute_error(y_train, y_predict_model_1_train)
model_1_mse_train = mean_squared_error(y_train, y_predict_model_1_train)
model_1_rmse_train = np.sqrt(model_1_mse_train)
model_1_r2_train = r2_score(y_train, y_predict_model_1_train)


print("Model_1 Training evaluation")
print("Mean Absolute Error:", model_1_mae_train)
print("Mean Squared Error:", model_1_mse_train)
print("Root Mean Squared Error:", model_1_rmse_train)
print("R-squared Score:", model_1_r2_train)

print()
```

```
Model_1 Training evaluation
Mean Absolute Error: 234.83182463454992
Mean Squared Error: 223887.45273241925
Root Mean Squared Error: 473.16746795655683
R-squared Score: 0.8747039104239243
```

In [51]:
```
# Model_1 Test evaluation

y_predict_model_1 = model_1_grid_search.predict(X_test)

model_1_mae = mean_absolute_error(y_test, y_predict_model_1)
model_1_mse = mean_squared_error(y_test, y_predict_model_1)
model_1_rmse = np.sqrt(model_1_mse)
model_1_r2 = r2_score(y_test, y_predict_model_1)


print("Model_1 Test evaluation")
print("Mean Absolute Error:", model_1_mae)
print("Mean Squared Error:", model_1_mse)
print("Root Mean Squared Error:", model_1_rmse)
print("R-squared Score:", model_1_r2)

print()
```

```
Model_1 Test evaluation
Mean Absolute Error: 234.1752678990775
Mean Squared Error: 159512.0249568771
Root Mean Squared Error: 399.38956540810767
R-squared Score: 0.9228177399040016
```

In [52]:
```
# Accuracy of the model
model_1_accuracy = model_1_grid_search.score(X_test, y_test)
model_1_accuracy
```

Out[52]:
```
0.9228177399040016
```

SVM

In [53]:
```
from sklearn.svm import SVR

# Create the SVR model
model_2 = SVR()

# Define the hyperparameters and their values to search over
model_2_param_grid = {
    'kernel': ['rbf','poly','sigmoid','linear'],
    'C': [0.1, 1, 10, 100, 1000],
    'gamma': ['scale', 'auto'],
    }

model_2_num_combination = 1

for model_2_k in model_2_param_grid.keys():
    model_2_num_combination *= len(model_2_param_grid[model_2_k])

print("Number of Combinations: ", model_2_num_combination)


# Perform grid search
model_2_grid_search = GridSearchCV(estimator=model_2, param_grid=model_2_par
model_2_grid_search.fit(X_train, y_train)
```

```
Number of Combinations:  40
```

Out[53]:
```
▸ GridSearchCV
▸ estimator: SVR
    ▸ SVR
```

In [54]:
```
# Get the best hyperparameters and the best model for model_3
model_2_best_params = model_2_grid_search.best_params_
model_2_best_model = model_2_grid_search.best_estimator_
```

In [55]:
```
model_2_best_params
```

Out[55]:
```
{'C': 1000, 'gamma': 'scale', 'kernel': 'poly'}
```

In [56]:
```
# Model_2 Train evaluation

y_predict_model_2_train = model_2_grid_search.predict(X_train)

model_2_mae_train = mean_absolute_error(y_train, y_predict_model_2_train)
model_2_mse_train = mean_squared_error(y_train, y_predict_model_2_train)
model_2_rmse_train = np.sqrt(model_2_mse_train)
model_2_r2_train = r2_score(y_train, y_predict_model_2_train)


print("Model_2 Train evaluation")
print("Mean Absolute Error:", model_2_mae_train)
print("Mean Squared Error:", model_2_mse_train)
print("Root Mean Squared Error:", model_2_rmse_train)
print("R-squared Score:", model_2_r2_train)

print()
```

```
Model_2 Train evaluation
Mean Absolute Error: 331.755898932371
Mean Squared Error: 584048.6471235857
Root Mean Squared Error: 764.2307551542176
R-squared Score: 0.6731437572151795
```

In [57]:
```
# Model_2 test evaluation
y_predict_model_2 = model_2_grid_search.predict(X_test)

model_2_mae = mean_absolute_error(y_test, y_predict_model_2)
model_2_mse = mean_squared_error(y_test, y_predict_model_2)
model_2_rmse = np.sqrt(model_2_mse)
model_2_r2 = r2_score(y_test, y_predict_model_2)


print("Model_2 test evaluation")
print("Mean Absolute Error:", model_2_mae)
print("Mean Squared Error:", model_2_mse)
print("Root Mean Squared Error:", model_2_rmse)
print("R-squared Score:", model_2_r2)

print()
```

```
Model_2 test evaluation
Mean Absolute Error: 312.2129615266444
Mean Squared Error: 345917.6031665916
Root Mean Squared Error: 588.147603214186
R-squared Score: 0.8326226350232466
```

In [58]:
```
# Accuracy of the model
model_2_accuracy = model_2_grid_search.score(X_test, y_test)
model_2_accuracy
```

Out[58]:
```
0.8326226350232466
```

KNeighborsRegressor

In [59]:
```
from sklearn.neighbors import KNeighborsRegressor

# Create the KNeighborsRegressor model
model_3 = KNeighborsRegressor()

# Define the hyperparameters and their values to search over
model_3_param_grid = {
    'n_neighbors': [1,3,5,7,9,11],
    'weights': ['uniform', 'distance'],
    'metric': ['minkowski','euclidean','manhattan'],
    'algorithm': ['auto', 'ball_tree', 'kd_tree', 'brute'],
    'leaf_size': [10, 20, 30, 40],
    'p': [1, 2]

}

model_3_num_combination = 1

for model_3_k in model_3_param_grid.keys():
    model_3_num_combination *= len(model_3_param_grid[model_3_k])

print("Number of Combinations: ", model_3_num_combination)


# Perform grid search
model_3_grid_search = GridSearchCV(estimator=model_3, param_grid=model_3_par
model_3_grid_search.fit(X_train, y_train)
```

```
Number of Combinations:  1152
```

Out[59]:
```
▸ GridSearchCV
▸ estimator: KNeighborsRegressor
  ▸ KNeighborsRegressor
```

In [60]:
```
# Get the best hyperparameters and the best model for model_4
model_3_best_params = model_3_grid_search.best_params_
model_3_best_model = model_3_grid_search.best_estimator_
```

In [61]:
```
model_3_best_params
```

Out[61]:
```
{'algorithm': 'ball_tree',
 'leaf_size': 10,
 'metric': 'minkowski',
 'n_neighbors': 3,
 'p': 1,
 'weights': 'uniform'}
```

In [62]:
```
# Model_3 Train evaluation

y_predict_model_3_train = model_3_grid_search.predict(X_train)

model_3_mae_train = mean_absolute_error(y_train, y_predict_model_3_train)
model_3_mse_train = mean_squared_error(y_train, y_predict_model_3_train)
model_3_rmse_train = np.sqrt(model_3_mse_train)
model_3_r2_train = r2_score(y_train, y_predict_model_3_train)


print("Model_3 Train evaluation")
print("Mean Absolute Error:", model_3_mae_train)
print("Mean Squared Error:", model_3_mse_train)
print("Root Mean Squared Error:", model_3_rmse_train)
print("R-squared Score:", model_3_r2_train)

print()
```

```
Model_3 Train evaluation
Mean Absolute Error: 153.65518566741585
Mean Squared Error: 118890.7839443876
Root Mean Squared Error: 344.80542911095176
R-squared Score: 0.9334641127358326
```

In [63]:
```
# test the model
y_predict_model_3 = model_3_grid_search.predict(X_test)

model_3_mae = mean_absolute_error(y_test, y_predict_model_3)
model_3_mse = mean_squared_error(y_test, y_predict_model_3)
model_3_rmse = np.sqrt(model_3_mse)
model_3_r2 = r2_score(y_test, y_predict_model_3)


print("Model_4 evaluation")
print("Mean Absolute Error:", model_3_mae)
print("Mean Squared Error:", model_3_mse)
print("Root Mean Squared Error:", model_3_rmse)
print("R-squared Score:", model_3_r2)

print()
```

```
Model_4 evaluation
Mean Absolute Error: 209.5362359395169
Mean Squared Error: 127534.29774995463
Root Mean Squared Error: 357.11944465396255
R-squared Score: 0.9382906376948159
```

In [64]:
```
# Accuracy of the model
model_3_accuracy = model_3_grid_search.score(X_test, y_test)
model_3_accuracy
```

Out[64]:
```
0.9382906376948159
```

GradientBoostingRegressor

In [65]:
```
from sklearn.ensemble import GradientBoostingRegressor

# Create the GradientBoostingRegressor model
model_4=GradientBoostingRegressor()

# Define the hyperparameters and their values to search over
model_4_param_grid = {
    'n_estimators': [3,5,10,20,40],
    'learning_rate': [0.01, 0.1, 0.5],
    'max_depth': [3, 5, 7],
    'min_samples_split': [2, 5, 10],
    'min_samples_leaf': [1, 2, 4],
    'max_features': ['auto', 'sqrt', 'log2',None]
}

model_4_num_combination = 1

for model_4_k in model_4_param_grid.keys():
    model_4_num_combination *= len(model_4_param_grid[model_4_k])

print("Number of Combinations: ", model_4_num_combination)

# Perform grid search
model_4_grid_search = GridSearchCV(estimator=model_4, param_grid=model_4_par
model_4_grid_search.fit(X_train, y_train)
```

```
Number of Combinations:  1620
```

Out[65]:
```
▸ GridSearchCV
▸ estimator: GradientBoostingRegressor
  ▸ GradientBoostingRegressor
```

In [66]:
```
# Get the best hyperparameters and the best model for model_2
model_4_best_params = model_4_grid_search.best_params_
model_4_best_model = model_4_grid_search.best_estimator_
```

In [67]:
```
model_4_best_params
```

Out[67]:
```
{'learning_rate': 0.5,
 'max_depth': 5,
 'max_features': 'sqrt',
 'min_samples_leaf': 1,
 'min_samples_split': 10,
 'n_estimators': 40}
```

In [68]:
```
# Model_4 train evaluation
y_predict_model_4_train = model_4_grid_search.predict(X_train)

model_4_mae_train = mean_absolute_error(y_train, y_predict_model_4_train)
model_4_mse_train = mean_squared_error(y_train, y_predict_model_4_train)
model_4_rmse_train = np.sqrt(model_4_mse_train)
model_4_r2_train = r2_score(y_train, y_predict_model_4_train)


print("Model_4 Train evaluation")
print("Mean Absolute Error:", model_4_mae_train)
print("Mean Squared Error:", model_4_mse_train)
print("Root Mean Squared Error:", model_4_rmse_train)
print("R-squared Score:", model_4_r2_train)

print()
```

```
Model_4 Train evaluation
Mean Absolute Error: 59.8707211419737
Mean Squared Error: 12712.591476786585
Root Mean Squared Error: 112.75012850008902
R-squared Score: 0.9928855414585327
```

In [69]:
```
# test the model
y_predict_model_4 = model_4_grid_search.predict(X_test)

model_4_mae = mean_absolute_error(y_test, y_predict_model_4)
model_4_mse = mean_squared_error(y_test, y_predict_model_4)
model_4_rmse = np.sqrt(model_4_mse)
model_4_r2 = r2_score(y_test, y_predict_model_4)


print("Model_4 Test evaluation")
print("Mean Absolute Error:", model_4_mae)
print("Mean Squared Error:", model_4_mse)
print("Root Mean Squared Error:", model_4_rmse)
print("R-squared Score:", model_4_r2)

print()
```

```
Model_4 Test evaluation
Mean Absolute Error: 200.47366712303446
Mean Squared Error: 106377.55639116574
Root Mean Squared Error: 326.1557241428789
R-squared Score: 0.948527640922499
```

XGBoost

In [70]:
```
import xgboost as xgb

# Create the XGBoost model
model_5 = xgb.XGBRegressor()

# Define the hyperparameters and their values to search over
model_5_param_grid = {
    'learning_rate': [0.01, 0.1, 0.5],
    'n_estimators': [100, 200, 300],
    'max_depth': [3, 5, 7],
    'reg_alpha': [0, 0.1, 1],
    'reg_lambda': [0, 0.1, 1],
    'subsample': [0.8, 1.0],
    'colsample_bytree': [0.8, 1.0],
    'gamma': [0, 0.1, 0.2]

}

model_5_num_combination = 1

for model_5_k in model_5_param_grid.keys():
    model_5_num_combination *= len(model_5_param_grid[model_5_k])

print("Number of Combinations: ", model_5_num_combination)


# Perform grid search
model_5_grid_search = GridSearchCV(estimator=model_5, param_grid=model_5_par
model_5_grid_search.fit(X_train, y_train)
```

```
Number of Combinations:  2916
```

Out[70]:
```
GridSearchCV
estimator: XGBRegressor
XGBRegressor
```

In [71]:
```
# Get the best hyperparameters and the best model for model_5
model_5_best_params = model_5_grid_search.best_params_
model_5_best_model = model_5_grid_search.best_estimator_
```

In [72]:
```
model_5_best_params
```

Out[72]:
```
{'colsample_bytree': 0.8,
 'gamma': 0,
 'learning_rate': 0.1,
 'max_depth': 3,
 'n_estimators': 300,
 'reg_alpha': 0.1,
 'reg_lambda': 0,
 'subsample': 1.0}
```

In [73]:
```
# Model_5 train evaluation
y_predict_model_5_train = model_5_grid_search.predict(X_train)

model_5_mae_train = mean_absolute_error(y_train, y_predict_model_5_train)
model_5_mse_train = mean_squared_error(y_train, y_predict_model_5_train)
model_5_rmse_train = np.sqrt(model_5_mse_train)
model_5_r2_train = r2_score(y_train, y_predict_model_5_train)


print("Model_5 Train evaluation")
print("Mean Absolute Error:", model_5_mae_train)
print("Mean Squared Error:", model_5_mse_train)
print("Root Mean Squared Error:", model_5_rmse_train)
print("R-squared Score:", model_5_r2_train)

print()
```

```
Model_5 Train evaluation
Mean Absolute Error: 65.51598101267386
Mean Squared Error: 13254.01179320743
Root Mean Squared Error: 115.12606912948705
R-squared Score: 0.9925825416805789
```

In [74]:
```
# Model_5 test evaluation
y_predict_model_5 = model_5_grid_search.predict(X_test)

model_5_mae = mean_absolute_error(y_test, y_predict_model_5)
model_5_mse = mean_squared_error(y_test, y_predict_model_5)
model_5_rmse = np.sqrt(model_5_mse)
model_5_r2 = r2_score(y_test, y_predict_model_5)


print("Model_5 test evaluation")
print("Mean Absolute Error:", model_5_mae)
print("Mean Squared Error:", model_5_mse)
print("Root Mean Squared Error:", model_5_rmse)
print("R-squared Score:", model_5_r2)

print()
```

```
Model_5 test evaluation
Mean Absolute Error: 212.9593244876682
Mean Squared Error: 134670.05909928257
Root Mean Squared Error: 366.9741940508659
R-squared Score: 0.9348378936863583
```

In [75]:
```
# Evaluate the model
accuracy = model_5_grid_search.score(X_test, y_test)
accuracy
```

Out[75]:
```
0.9348378936863583
```

RESULT

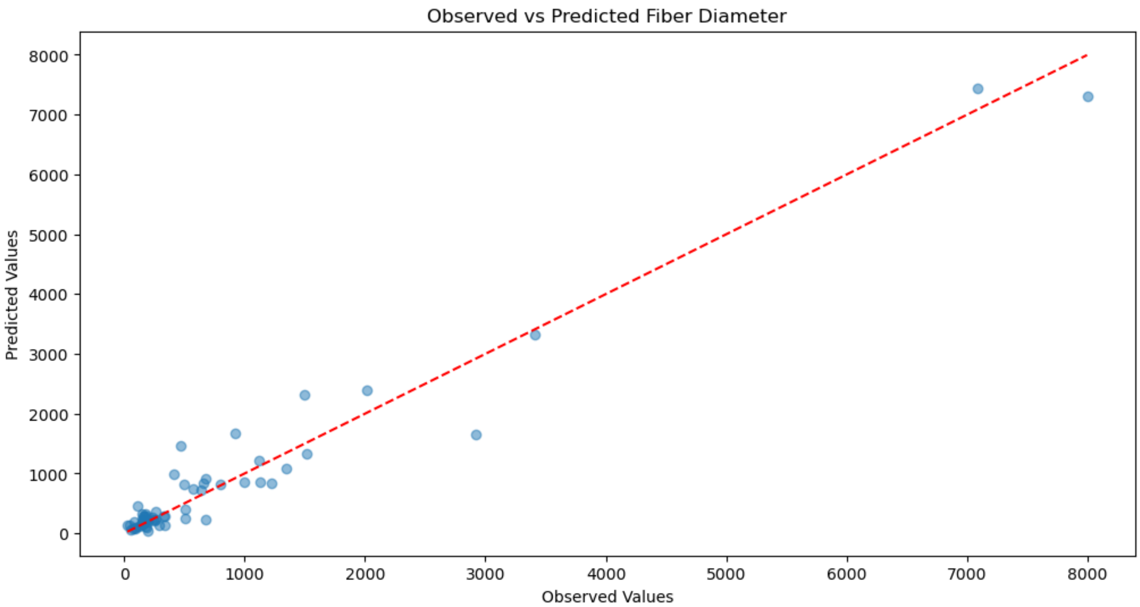
In [76]:
```
rows = []

model_name=["RandomForestRegressor","SVM","KNeighborsRegressor","GradientBoo

# Loop through the range 1 to 5
for i in range(1, 6):
    # Assign values to model-specific variables
    model_mae = f"model_{i}_mae"
    model_mse = f"model_{i}_mse"
    model_rmse = f"model_{i}_rmse"
    model_r2 = f"model_{i}_r2"
    model_best_params = f"model_{i}_best_params"

    # Create a dictionary for the model performance metrics
    performance_dict = {
        'Model': model_name[i-1],
        'Mean Absolute Error (MAE)': eval(model_mae),
        'Mean Squared Error (MSE)': eval(model_mse),
        'Root Mean Squared Error (RMSE)': eval(model_rmse),
        'R-squared Score': eval(model_r2),
        'Best Hyperparameters': eval(model_best_params)
    }

    # Append the performance dictionary to the list
    rows.append(performance_dict)

# Convert the list of dictionaries into a DataFrame
performance_df = pd.DataFrame(rows)
```

In [77]:
```
performance_df
```

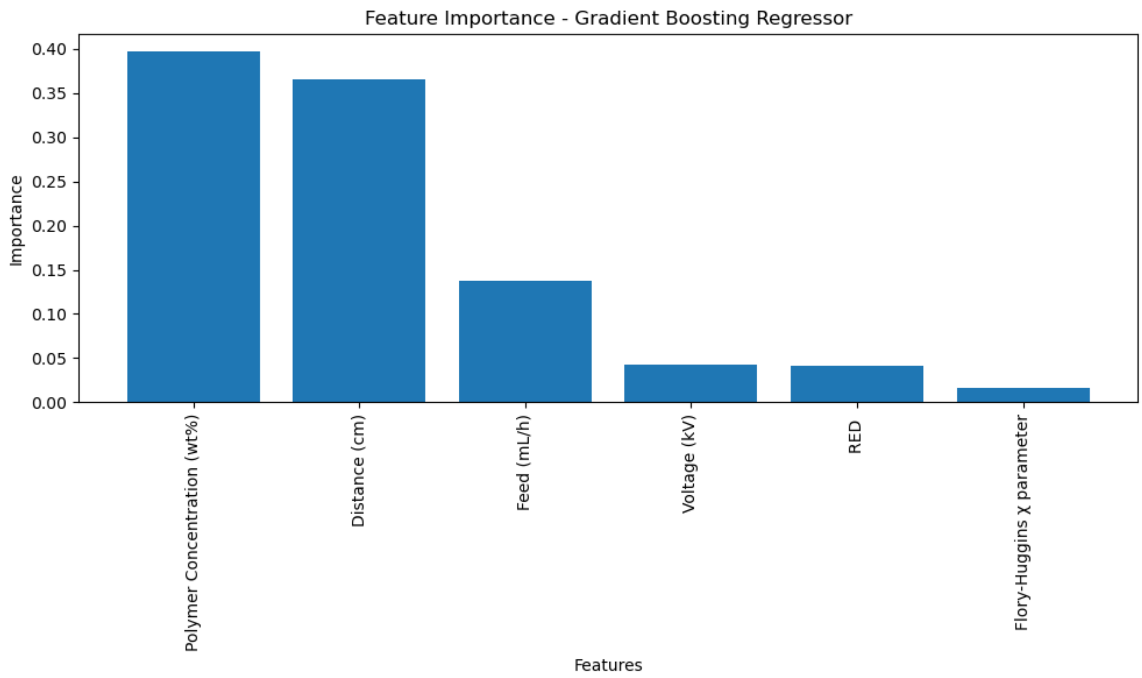
Out[77]:

	Model	Mean Absolute Error (MAE)	Mean Squared Error (MSE)	Root Mean Squared Error (RMSE)	R-squared Score	B Hyperparamet
0	RandomForestRegressor	234.175268	159512.024957	399.389565	0.922818	{'max_depth': 'max_featur 'log2', 'mi
1	SVM	312.212962	345917.603167	588.147603	0.832623	{'C': 1000, 'gamn 'scale', 'kerr 'pc
2	KNeighborsRegressor	209.536236	127534.297750	357.119445	0.938291	{'algorith 'ball_tr 'leaf_size': 10, 'r
3	GradientBoostingRegressor	200.473667	106377.556391	326.155724	0.948528	{'learning_rate': ('max_depth' 'max_f
4	XGBRegressor	212.959324	134670.059099	366.974194	0.934838	{'colsample_bytr 0.8, 'gamma' 'learni

In [80]:
```
import matplotlib.pyplot as plt


# Create a scatter plot of observed versus predicted values
plt.scatter(y_test, y_predict_model_4, alpha=0.5)
plt.xlabel('Observed Values')
plt.ylabel('Predicted Values')
plt.title('Observed vs Predicted Fiber Diameter')

# Add a diagonal line for reference (perfect predictions)
plt.plot([min(y_test), max(y_test)], [min(y_test), max(y_test)], 'r--')

# Show the plot
plt.show()
```



In [81]:
```
import numpy as np
import matplotlib.pyplot as plt

# Train the XGBoost Regressor model
model = GradientBoostingRegressor(**model_4_best_params)
model.fit(X_train, y_train)

# Get the feature importances
importances = model.feature_importances_
features = X_train.columns

# Sort feature importances in descending order
indices = np.argsort(importances)[::-1]

# Plot the feature importances
plt.figure(figsize=(10, 6))
plt.title("Feature Importance - Gradient Boosting Regressor")
plt.bar(range(len(importances)), importances[indices], align="center")
plt.xticks(range(len(importances)), [features[i] for i in indices], rotatior
plt.xlabel("Features")
plt.ylabel("Importance")
plt.tight_layout()

# Show the plot
plt.show()
```



In [ ]: