In [4]:
```
pip install numpy pandas matplotlib seaborn scikit-learn xgboost
```

```
Requirement already satisfied: numpy in c:\users\dgous\anaconda3\lib\site-pac
kages (1.24.3)
Requirement already satisfied: pandas in c:\users\dgous\anaconda3\lib\site-pa
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e-packages (3.7.1)
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ackages (0.12.2)
Requirement already satisfied: scikit-learn in c:\users\dgous\anaconda3\lib\s
ite-packages (1.4.1.post1)
Requirement already satisfied: xgboost in c:\users\dgous\anaconda3\lib\site-p
ackages (2.0.3)
Requirement already satisfied: python-dateutil>=2.8.1 in c:\users\dgous\anaco
nda3\lib\site-packages (from pandas) (2.8.2)
Requirement already satisfied: pytz>=2020.1 in c:\users\dgous\anaconda3\lib\s
ite-packages (from pandas) (2022.7)
Requirement already satisfied: contourpy>=1.0.1 in c:\users\dgous\anaconda3\l
ib\site-packages (from matplotlib) (1.0.5)
Requirement already satisfied: cycler>=0.10 in c:\users\dgous\anaconda3\lib\s
ite-packages (from matplotlib) (0.11.0)
Requirement already satisfied: fonttools>=4.22.0 in c:\users\dgous\anaconda3
\lib\site-packages (from matplotlib) (4.25.0)
Requirement already satisfied: kiwisolver>=1.0.1 in c:\users\dgous\anaconda3
\lib\site-packages (from matplotlib) (1.4.4)
Requirement already satisfied: packaging>=20.0 in c:\users\dgous\anaconda3\li
b\site-packages (from matplotlib) (23.0)
Requirement already satisfied: pillow>=6.2.0 in c:\users\dgous\anaconda3\lib
\site-packages (from matplotlib) (9.4.0)
Requirement already satisfied: pyparsing>=2.3.1 in c:\users\dgous\anaconda3\l
ib\site-packages (from matplotlib) (3.0.9)
Requirement already satisfied: scipy>=1.6.0 in c:\users\dgous\anaconda3\lib\s
ite-packages (from scikit-learn) (1.10.1)
Requirement already satisfied: joblib>=1.2.0 in c:\users\dgous\anaconda3\lib
\site-packages (from scikit-learn) (1.2.0)
Requirement already satisfied: threadpoolctl>=2.0.0 in c:\users\dgous\anacond
a3\lib\site-packages (from scikit-learn) (2.2.0)
Requirement already satisfied: six>=1.5 in c:\users\dgous\anaconda3\lib\site-
packages (from python-dateutil>=2.8.1->pandas) (1.16.0)
Note: you may need to restart the kernel to use updated packages.
```

In [5]:
```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
from sklearn.model_selection import train_test_split
from sklearn.ensemble import RandomForestRegressor
from xgboost import XGBRegressor
from sklearn.decomposition import PCA
from sklearn.linear_model import LinearRegression
from sklearn.preprocessing import StandardScaler
```

In [6]:
```
np.random.seed(42)
num_samples = 100  # Reduced from 500 to 100

# Generate synthetic formulation data
excipient_ratio = np.random.uniform(0.1, 1.0, num_samples)
compression_force = np.random.uniform(5, 50, num_samples)
granule_size = np.random.uniform(100, 500, num_samples)
binder_percentage = np.random.uniform(1, 10, num_samples)

# Target Variables (Dependent Variables)
dissolution_profile = 10 + 3*excipient_ratio + 1.5*compression_force - 0.01*gr
bioavailability = 20 + 4*excipient_ratio - 0.5*compression_force + 0.02*granul

# Create DataFrame
df = pd.DataFrame({
    "Excipient Ratio": excipient_ratio,
    "Compression Force": compression_force,
    "Granule Size": granule_size,
    "Binder Percentage": binder_percentage,
    "Dissolution Profile": dissolution_profile,
    "Bioavailability": bioavailability
})

# Display first few rows
print(df.head())
```

```
   Excipient Ratio  Compression Force  Granule Size  Binder Percentage  \
0         0.437086           6.414313    356.812658           1.465135
1         0.955643          33.638469    133.655986           5.782192
2         0.758795          19.146019    164.651486           5.865716
3         0.638793          27.885681    459.421675           6.736869
4         0.240417          45.840491    342.571624           7.534822

   Dissolution Profile  Bioavailability
0            19.975559        26.674383
1            62.030079         7.430997
2            40.712803        21.408654
3            48.530149        18.147787
4            76.704604         8.430745
```

In [7]:
```
X = df[["Excipient Ratio", "Compression Force", "Granule Size", "Binder Percer
y_dissolution = df["Dissolution Profile"]
y_bioavailability = df["Bioavailability"]

# Split the data
X_train, X_test, y_train_dissolution, y_test_dissolution = train_test_split(X,
X_train, X_test, y_train_bioavailability, y_test_bioavailability = train_test_
```

In [8]:
```
rf_model = RandomForestRegressor(n_estimators=10, random_state=42)  # Reduced
rf_model.fit(X_train, y_train_dissolution)
rf_pred = rf_model.predict(X_test)

print("Random Forest Model trained successfully for Dissolution Profile Predic
```

```
Random Forest Model trained successfully for Dissolution Profile Prediction
```

In [9]:
```
xgb_model = XGBRegressor(n_estimators=5, random_state=42)  # Reduced estimator
xgb_model.fit(X_train, y_train_bioavailability)
xgb_pred = xgb_model.predict(X_test)

print("XGBoost Model trained successfully for Bioavailability Prediction")
```

```
XGBoost Model trained successfully for Bioavailability Prediction
```

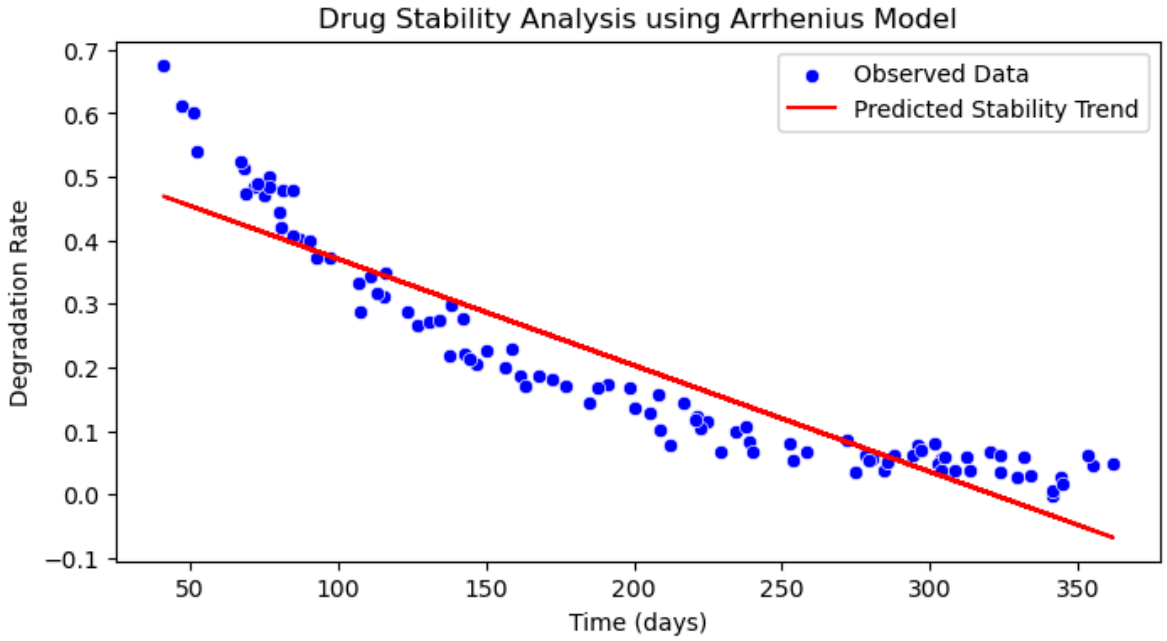
In [10]:
```
scaler = StandardScaler()
X_scaled = scaler.fit_transform(X)
pca = PCA(n_components=2)
X_pca = pca.fit_transform(X_scaled)
df_pca = pd.DataFrame(X_pca, columns=["PC1", "PC2"])

print("PCA Analysis Completed")
```

```
PCA Analysis Completed
```

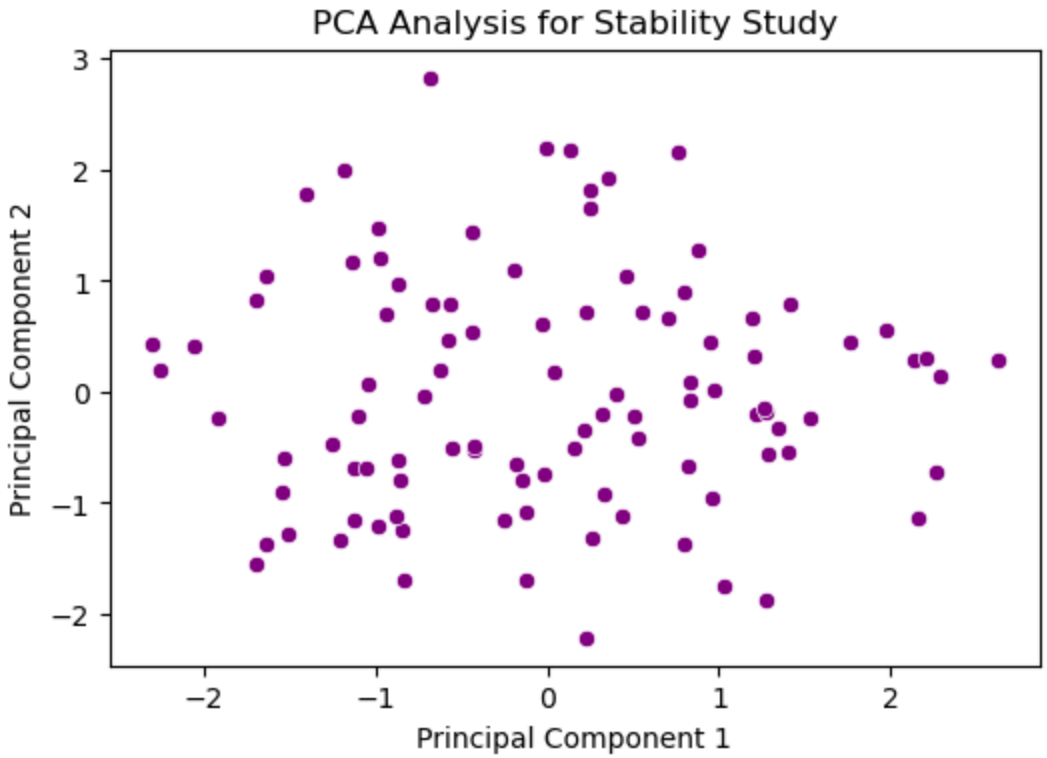
In [11]:
```
stability_time = np.random.uniform(30, 365, num_samples)
degradation_rate = np.exp(-0.01 * stability_time) + np.random.normal(0, 0.02,

X_stability = stability_time.reshape(-1, 1)
y_stability = degradation_rate

reg_model = LinearRegression()
reg_model.fit(X_stability, y_stability)
stability_pred = reg_model.predict(X_stability)

print("Regression Model trained for Drug Stability Analysis")
```

```
Regression Model trained for Drug Stability Analysis
```

In [12]:
```
plt.figure(figsize=(8,4))
sns.scatterplot(x=stability_time, y=degradation_rate, label="Observed Data", c
plt.plot(stability_time, stability_pred, color="red", label="Predicted Stabili
plt.xlabel("Time (days)")
plt.ylabel("Degradation Rate")
plt.title("Drug Stability Analysis using Arrhenius Model")
plt.legend()
plt.show()
```



In [13]:
```
plt.figure(figsize=(6,4))
sns.scatterplot(x=df_pca["PC1"], y=df_pca["PC2"], color="purple")
plt.xlabel("Principal Component 1")
plt.ylabel("Principal Component 2")
plt.title("PCA Analysis for Stability Study")
plt.show()
```



In [ ]: