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

In [2]:
```python
# importing dataset
df = pd.read_csv('/content/Concrete_Data_Yeh.csv')
df.head()
```

Out[2]:

	cement	slag	flyash	water	superplasticizer	coarseaggregate	fineaggrega
0	540.0	0.0	0.0	162.0	2.5	1040.0	676
1	540.0	0.0	0.0	162.0	2.5	1055.0	676
2	332.5	142.5	0.0	228.0	0.0	932.0	594
3	332.5	142.5	0.0	228.0	0.0	932.0	594
4	198.6	132.4	0.0	192.0	0.0	978.4	825

In [3]:
```python
df.shape
```

Out[3]: (1030, 9)

In [4]:
```python
df.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 1030 entries, 0 to 1029
Data columns (total 9 columns):
 #   Column            Non-Null Count  Dtype  
---  ------            --------------  -----  
 0   cement            1030 non-null   float64
 1   slag              1030 non-null   float64
 2   flyash            1030 non-null   float64
 3   water             1030 non-null   float64
 4   superplasticizer  1030 non-null   float64
 5   coarseaggregate   1030 non-null   float64
 6   fineaggregate     1030 non-null   float64
 7   age               1030 non-null   int64  
 8   csMPa             1030 non-null   float64
dtypes: float64(8), int64(1)
memory usage: 72.6 KB
```

The dataset is clean, fully numeric, and domain-driven, making it ideal for regression modeling. However, the small sample size and expected non-linear interactions require careful validation and conservative model complexity.

In [5]:
```python
df.describe()
```

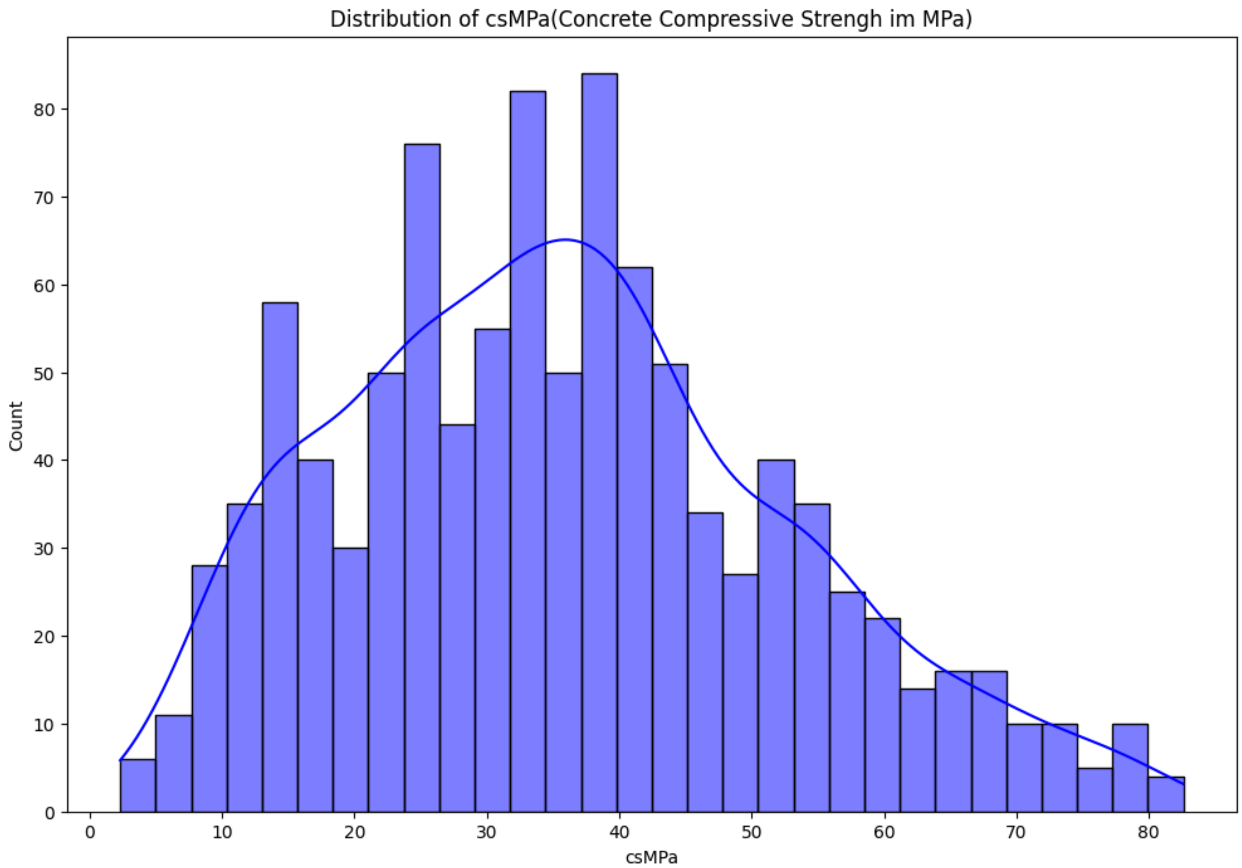
Out[5]:

	cement	slag	flyash	water	superplasticizer	coa
count	1030.000000	1030.000000	1030.000000	1030.000000	1030.000000	
mean	281.167864	73.895825	54.188350	181.567282	6.204660	
std	104.506364	86.279342	63.997004	21.354219	5.973841	
min	102.000000	0.000000	0.000000	121.800000	0.000000	
25%	192.375000	0.000000	0.000000	164.900000	0.000000	
50%	272.900000	22.000000	0.000000	185.000000	6.400000	
75%	350.000000	142.950000	118.300000	192.000000	10.200000	
max	540.000000	359.400000	200.100000	247.000000	32.200000	

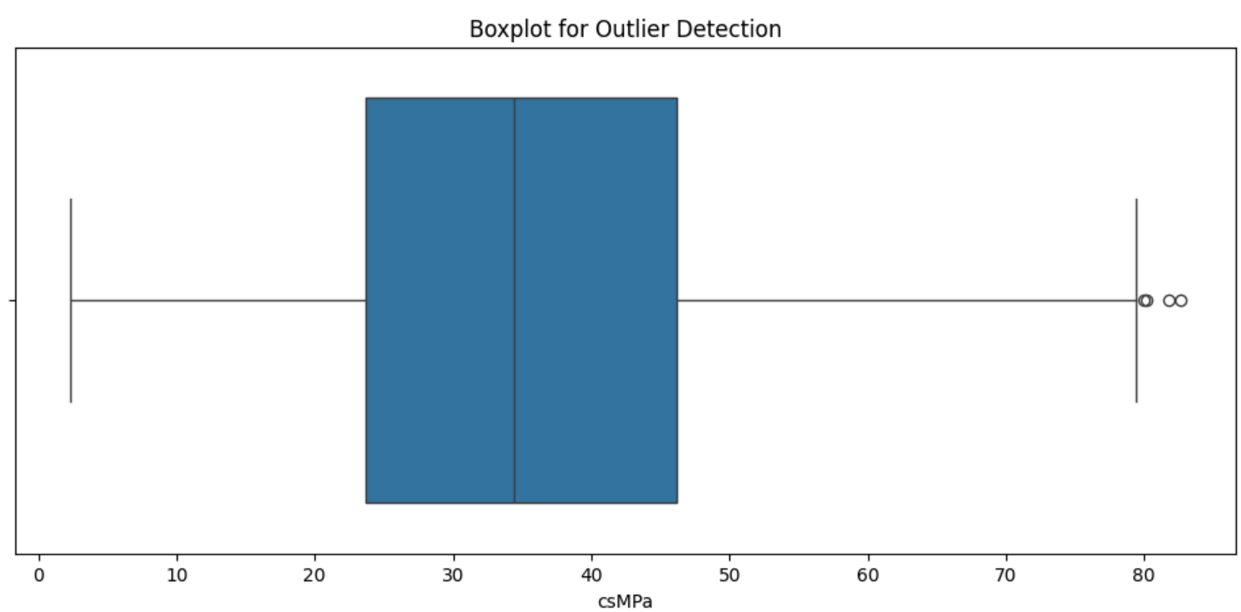
The dataset shows high variability and strong skewness across key material components and curing age, indicating non-linear relationships and interaction effects that favor tree-based regression models over linear approaches.

In [6]:

```
# Target distribution
plt.figure(figsize=(12,8))
sns.histplot(df['csMPa'], kde=True, color='blue', bins=30)
plt.title('Distribution of csMPa(Concrete Compressive Strengh im MPa)')
plt.xlabel('csMPa')
plt.show()
```



In [7]:
```
# Outliers
plt.figure(figsize=(12,5))
sns.boxplot(data=df, x='csMPa')
plt.title('Boxplot for Outlier Detection')
plt.show()
```

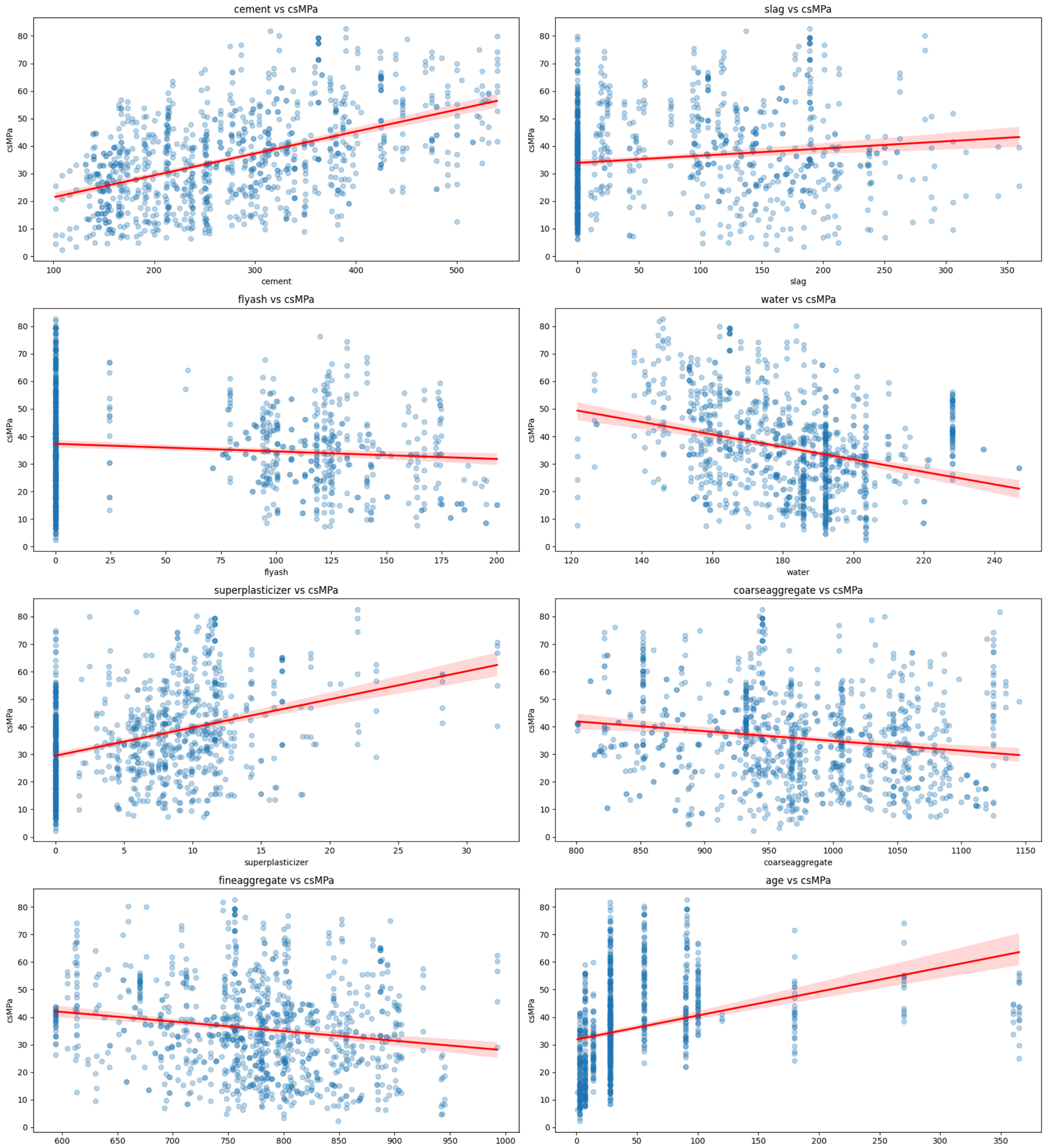


The target variable exhibits a right-skewed distribution with a small number of high-strength outliers that are physically meaningful. These observations are retained, as they reflect real high-performance concrete mixes and are essential for realistic model behavior

In [8]:
```
len(df.columns)
```

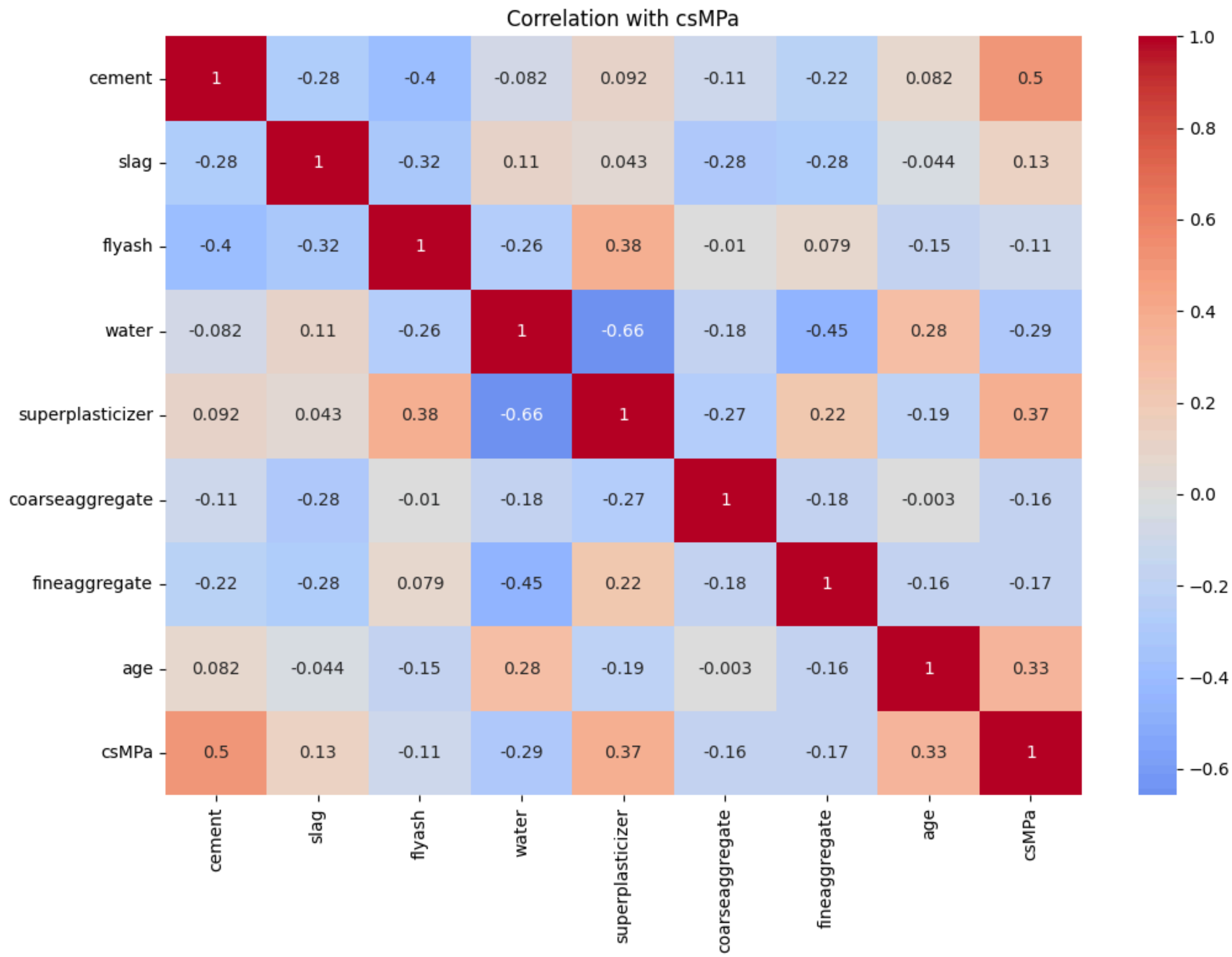
Out[8]: 9

In [9]:
```
# Scatter Plots with regression lines
feature_cols = df.columns.drop('csMPa')

fig, axes = plt.subplots(nrows=4, ncols=2, figsize=(18,20))
axes = axes.flatten()
for ax, col in zip(axes, feature_cols):
  sns.regplot(data=df, x=col, y='csMPa', ax=ax, scatter_kws={'alpha':0.3}, lir
  ax.set_title(f'{col} vs csMPa')

plt.tight_layout()
plt.show()
```



Scatter plots highlight interaction-driven effects, particularly between water, cement, and superplasticizer, reinforcing the suitability of tree-based regression models for this dataset

In [10]:
```
# # Calculating correlation
corr = df.corr()
plt.figure(figsize=(12,8))
sns.heatmap(corr, annot=True, cmap='coolwarm', center=0)
plt.title('Correlation with csMPa')
plt.show()
```



Correlation analysis reveals cement as the strongest linear predictor of compressive strength, while age and superplasticizer exhibit moderate correlations that understate their true non-linear influence

Model Building

In [11]:
```
# sikit-learn libraries
from sklearn.model_selection import train_test_split
from sklearn.linear_model import LinearRegression
from sklearn.ensemble import RandomForestRegressor
from sklearn.model_selection import RandomizedSearchCV
from sklearn.metrics import r2_score, mean_squared_error, mean_absolute_error
```

In [12]:
```
# Spliting DataFrame into X and y (Features and Target)
X = df.drop(columns='csMPa')
y = df['csMPa']

# Train/Test split (80%/20%)
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, rando
```

In [13]:
```
X_train.shape, X_test.shape
```

Out[13]:
```
((824, 8), (206, 8))
```

In [14]:
```
# Creating a baseline Linear Regression model to compare with out Random Fores
lr = LinearRegression()
lr.fit(X_train, y_train)

y_pred_lr = lr.predict(X_test)
rmse_lr = np.sqrt(mean_squared_error(y_test, y_pred_lr))

print('Linear Regression Test R2:', lr.score(X_test, y_test))
print('Linear Regression R2:', r2_score(y_test, y_pred_lr))
print('Linear Regression RMSE', rmse_lr)
print("Linear Regression MAE:", mean_absolute_error(y_test, y_pred_lr))
```

```
Linear Regression Test R2: 0.627553179231485
Linear Regression R2: 0.627553179231485
Linear Regression RMSE 9.796475901624358
Linear Regression MAE: 7.745559243921434
```

In [15]:
```
# Random Forest Regression model
rf = RandomForestRegressor(n_estimators=500, random_state=42, n_jobs=-1, oob_s
rf.fit(X_train, y_train)

y_pred_rf = rf.predict(X_test)

print('OOB R2:', rf.oob_score_)
print('Random Forest Test R2:', rf.score(X_test, y_test))
```

```
OOB R2: 0.9165366789063125
Random Forest Test R2: 0.882997006966324
```

In [16]:
```
min_leaf_values = [1, 3, 5, 10, 20]

for leaf in min_leaf_values:
    rf.set_params(min_samples_leaf=leaf)
    rf.fit(X_train, y_train)
    print(f'leaf:{leaf}, OOB R2: {rf.oob_score_}, r2_score:{r2_score(y_test, r
```

```
leaf:1, OOB R2: 0.9165366789063125, r2_score:0.882997006966324
leaf:3, OOB R2: 0.9023874082295817, r2_score:0.8680847041066069
leaf:5, OOB R2: 0.8868071637752885, r2_score:0.855068662323721
leaf:10, OOB R2: 0.8532620848776744, r2_score:0.8203061601295569
leaf:20, OOB R2: 0.8001082554321509, r2_score:0.756722705398591
```

Based on the experiment and results, `min_samples_leaf=1` is the best choice in terms of predictive performance, while `min_samples_leaf=3` offers a more conservative bias–variance trade-off with minimal loss in accuracy.

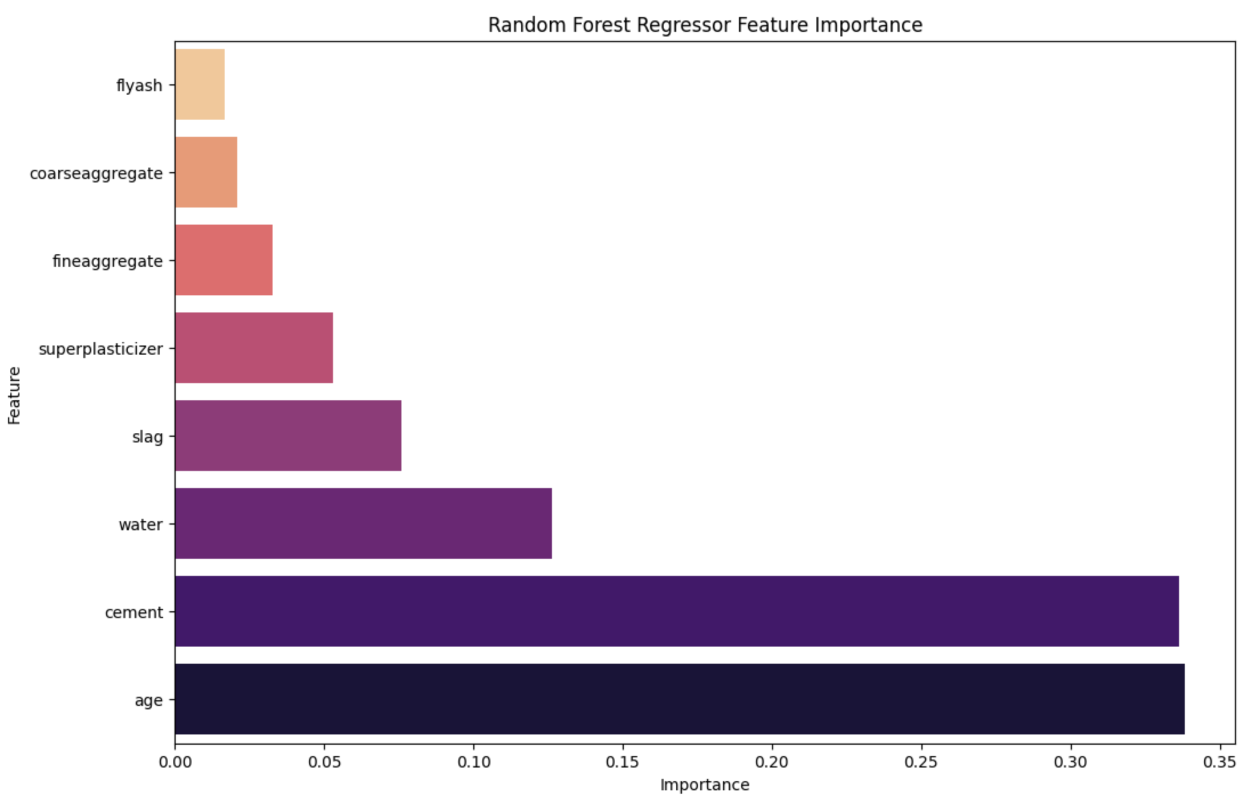
In [17]:
```
# Final Random forest model
rf_final = RandomForestRegressor(n_estimators=500, min_samples_leaf=3, random_
```

```
rf_final.fit(X_train, y_train)
y_pred_rf_final = rf_final.predict(X_test)
rmse_rf = np.sqrt(mean_squared_error(y_test, y_pred_rf_final))

print("Final OOB R²:", rf_final.oob_score_)
print("Final Test R²:", rf_final.score(X_test, y_test))
print('Random Forest RMSE:', rmse_rf)
print('Random Forest MAE:', mean_absolute_error(y_test, y_pred_rf_final))
```

```
Final OOB R²: 0.9023874082295817
Final Test R²: 0.8680847041066069
Random Forest RMSE: 5.83022501836955
Random Forest MAE: 4.256993399793737
```

In [18]:

```
# Feature names and Importance
importances = rf_final.feature_importances_
feature_name = X_train.columns

# Converting to DataFrame
fi_df = pd.DataFrame({
    'Feature': feature_name,
    'Importance': importances
}).sort_values(by='Importance', ascending=False)

plt.figure(figsize=(12,8))
sns.barplot(data=fi_df, x='Importance', y='Feature', hue='Feature', palette='m
plt.gca().invert_yaxis()
plt.title('Random Forest Regressor Feature Importance')
plt.xlabel('Importance')
plt.show()
```



Feature importance analysis from the Random Forest model indicates that curing age and cement content are the dominant predictors of compressive strength, followed by water content. Supplementary materials such as slag and superplasticizer exhibit moderate importance, reflecting their interaction-driven effects. Aggregates and fly ash contribute less to predictive performance. These results align closely with both exploratory analysis and domain knowledge, supporting the validity of the model.

Final Project Conclusion & Limitations

Final Conclusion

This project aimed to predict **concrete compressive strength (`csMPa`)** using mix composition and curing age, leveraging both exploratory data analysis and machine learning models. The dataset was found to be **clean**, **fully numerical**, and **domain-driven**, with no missing values or categorical variables, allowing the analysis to focus on understanding underlying relationships rather than preprocessing challenges.

Exploratory Data Analysis (EDA)

Exploratory Data Analysis revealed that the relationships between input features and compressive strength are **strongly non-linear** and **interaction-driven**, particularly involving cement content, curing age, water, and superplasticizer. Linear assumptions were shown to be insufficient, as confirmed by weak linear fits and moderate Pearson correlations that underestimated the true influence of several key variables.

Modeling Approach and Performance

A **Linear Regression** model was established as a baseline, achieving a **test R^2** of approximately **0.63** with relatively high prediction error. While interpretable, this model failed to capture the complex non-linear behavior inherent in concrete strength development.

In contrast, a **Random Forest Regressor** with **Out-of-Bag (OOB) validation** significantly improved performance. The final model achieved a **Test R^2 of ~0.87**, reducing RMSE from nearly **10 MPa** to **~5.8 MPa** and MAE from **~7.7 MPa** to **~4.2 MPa**, demonstrating a substantial and meaningful improvement in predictive accuracy. The close alignment between OOB R^2 (~0.90) and test R^2 further indicates strong generalization and minimal overfitting.

Feature Importance Analysis

Feature importance analysis showed that **curing age** and **cement content** are the dominant predictors of compressive strength, followed by **water content**. Supplementary materials such as **slag** and **superplasticizer** exhibited moderate importance, reflecting their interaction-driven effects, while aggregates and fly ash contributed less to predictive performance. These findings are consistent with both exploratory analysis and established domain knowledge, reinforcing the credibility of the model.

Project Concution

Overall, this project demonstrates that **tree-based models are well-suited for modeling concrete compressive strength**, where non-linearity, feature interactions, and physical constraints play a central role. The final Random Forest model provides a robust, interpretable, and practically useful solution without relying on aggressive hyperparameter tuning.

Limitations & Future Work

Despite its strong performance, this study has several important limitations:

1. **Dataset Size:** The dataset contains only ~1,000 samples. While sufficient for Random Forest modeling, this limits the model's ability to generalize to rare or extreme mix designs and increases sensitivity to data splits.

2. **Lack of External Validation:** Model performance was evaluated using a train–test split and OOB estimation within the same dataset. Performance on completely independent datasets or real-world production data remains untested.

3. **No Explicit Ratio Features:** Important domain concepts such as the water–cement ratio were learned implicitly by the model rather than being explicitly engineered. Incorporating such features could improve interpretability and potentially performance.

4. **Limited Extrapolation Ability:** Random Forest models do not extrapolate well beyond the observed data range. Predictions for very high-strength concrete or unusual curing ages should be interpreted cautiously.

5. **Interpretability Constraints:** While feature importance provides insight into model behavior, it does not establish causality or directionality. More advanced explainability techniques (e.g., SHAP values or partial dependence plots) could further enhance interpretability.

Final Takeaway

This project successfully shows that **model choice must be driven by data characteristics**, not convenience. By grounding modeling decisions in EDA, prioritizing generalization over over-tuning, and validating results carefully, the final Random Forest model delivers **strong**, **realistic**, and **defensible predictions** of concrete compressive strength. The approach and conclusions are suitable for both practical applications and technical evaluation in interviews or academic settings.

In [18]:

```

```