TNFA-XGBoost
seed: 793
Best Parameters: {'colsample_bytree': 0.9, 'learning_rate': 0.1, 'max_depth': 4, 'n_estimators': 200, 'reg_alpha': 0.1, 'reg_lambda': 1.5, 'subsample': 0.9}
R^2 on test set (log scale): 0.7347
R^2 on training set (original scale): 0.9946
R^2 on test set (original scale): 0.9023
Test MSE: 21294.32
Test MAE: 77.21
Test MAPE (%): 37.53

seed: 235
Best Parameters: {'colsample_bytree': 0.9, 'learning_rate': 0.1, 'max_depth': 5, 'n_estimators': 200, 'reg_alpha': 0.1, 'reg_lambda': 1, 'subsample': 0.8}
R^2 on test set (log scale): 0.7868
R^2 on training set (original scale): 0.9970
R^2 on test set (original scale): 0.9302
Test MSE: 28882.16
Test MAE: 108.15
Test MAPE (%): 33.05

seed: 42
Best Parameters: {'colsample_bytree': 0.8, 'learning_rate': 0.1, 'max_depth': 3, 'n_estimators': 300, 'reg_alpha': 0.1, 'reg_lambda': 1.5, 'subsample': 0.8}
R^2 on test set (log scale): 0.5003
R^2 on training set (original scale): 0.9919
R^2 on test set (original scale): 0.9540
Test MSE: 17821.68
Test MAE: 80.93
Test MAPE (%): 86.50

Average Test R^2 (original scale): 0.9288 ± 0.0259
Average Test R^2 (log scale): 0.6740 ± 0.1526
Average Test MSE: 22666.05 ± 5656.39
Average Test MAE: 88.76 ± 16.89
Average Test MAPE (%): 52.36 ± 29.65

TNFA-RF
seed: 42
Best Parameters: {'bootstrap': True, 'max_depth': 20, 'max_features': 'sqrt', 'min_samples_leaf': 1, 'min_samples_split': 2, 'n_estimators': 500}
R^2 on test set (log scale) : 0.6951
R^2 on training set (original scale): 0.9011
R^2 on test set (original scale): 0.9050
Test MSE: 36821.31
Test MAE: 118.47
Test MAPE (%): 109.13

seed: 793
Best Parameters: {'bootstrap': True, 'max_depth': 10, 'max_features': 'sqrt', 'min_samples_leaf': 1, 'min_samples_split': 2, 'n_estimators': 300}
R^2 on test set (log scale): 0.7739
R^2 on training set (original scale): 0.8832
R^2 on test set (original scale): 0.8091
Test MSE: 41617.48
Test MAE: 106.03
Test MAPE (%): 38.50

seed: 235
Best Parameters: {'bootstrap': True, 'max_depth': None, 'max_features': 'sqrt', 'min_samples_leaf': 1, 'min_samples_split': 2, 'n_estimators': 300}
R^2 on test set (log scale): 0.7641
R^2 on test set (original scale): 0.8705
R^2 on test set (original scale): 0.8291
Test MSE: 70668.69
Test MAE: 155.35
Test MAPE (%): 44.31

Average Test R^2 (original scale): 0.8478 ± 0.0506
Average Test R^2 (log scale): 0.7443 ± 0.0429
Average Test MSE: 49702.50 ± 18314.93
Average Test MAE: 126.62 ± 25.65
Average Test MAPE (%): 63.98 ± 39.21

TNFA-MLP
seed: 42
Best Parameters: {'reg__regressor__activation': 'relu', 'reg__regressor__alpha': 0.0005, 'reg__regressor__batch_size': 64, 'reg__regressor__hidden_layer_sizes': (128, 64), 'reg__regressor__learning_rate_init': 0.0005, 'reg__regressor__solver': 'adam'}
R^2 on test set (log scale): 0.6606
R^2 on training set (original scale): 0.8254
R^2 on test set (original scale): 0.9162
Test MSE: 32506.24
Test MAE: 117.35
Test MAPE (%): 126.93

seed: 793
Best Parameters: {'reg__regressor__activation': 'relu', 'reg__regressor__alpha': 0.0005, 'reg__regressor__batch_size': 32, 'reg__regressor__hidden_layer_sizes': (128, 64), 'reg__regressor__learning_rate_init': 0.0005, 'reg__regressor__solver': 'adam'}
R^2 on test set (log scale): 0.6316
R^2 on training set (original scale): 0.6680
R^2 on test set (original scale): 0.7650
Test MSE: 51234.92
Test MAE: 126.95
Test MAPE (%): 52.98

seed: 1579
Best Parameters: {'reg__regressor__activation': 'relu', 'reg__regressor__alpha': 0.0005, 'reg__regressor__batch_size': 32, 'reg__regressor__hidden_layer_sizes': (256, 128, 64), 'reg__regressor__learning_rate_init': 0.0005, 'reg__regressor__solver': 'adam'}
R^2 on test set (log scale): 0.6906
R^2 on training set (original scale): 0.7927
R^2 on test set (original scale): 0.6654
Test MSE: 116024.54
Test MAE: 214.31
Test MAPE (%): 68.81

========= Mean ± Std (Test Set, Original Scale) =========
Average Test R^2 (original scale): 0.7822 ± 0.1263
Average Test R^2 (log scale): 0.6609 ± 0.0295
Average Test MSE: 66588.57 ± 43824.96
Average Test MAE: 152.87 ± 53.43
Average Test MAPE (%): 82.91 ± 38.94

IL-10 XGBoost
Running with random seed: 42
Train R^2: 0.8862
Test R^2: 0.7077
Test MSE: 29216.08
Test MAE: 109.46
Test MAPE (%): 37.78

Running with random seed: 173
Train R^2: 0.8567
Test R^2: 0.8111
Test MSE: 18360.08

Test MAE: 96.34
Test MAPE (%): 66.50

Running with random seed: 382
Train R²: 0.8503
Test R²: 0.8309
Test MSE: 20670.59
Test MAE: 94.96
Test MAPE (%): 70.26

Average Test R²: 0.7832 ± 0.0662
Average Test MSE: 22748.92 ± 5718.63
Average Test MAE: 100.25 ± 8.01
Average Test MAPE (%): 58.18 ± 17.76

IL-10 RF
Running with random seed: 1
Train R²: 0.8238
Test R²: 0.8075
Test MSE: 23635.01
Test MAE: 123.03
Test MAPE (%): 86.92

Running with random seed: 173
Train R²: 0.8101
Test R²: 0.8276
Test MSE: 16753.27
Test MAE: 116.62
Test MAPE (%): 116.28

Running with random seed: 98
Train R²: 0.8028
Test R²: 0.7368
Test MSE: 41253.77
Test MAE: 152.62
Test MAPE (%): 93.95

Average Test R²: 0.7907 ± 0.0477
Average Test MSE: 27214.02 ± 12636.29
Average Test MAE: 130.75 ± 19.20
Average Test MAPE (%): 99.05 ± 15.33

IL-10 MLP
Running with seed: 79
R² on test set (log/transformed scale): 0.3012
R² on training set (original scale): 0.9206
R² on test set (original scale): 0.7377
Test MSE: 699181.58
Test MAE: 427.93
Test MAPE (%): 188.35
Best Parameters: {'reg__regressor__activation': 'relu', 'reg__regressor__alpha': 0.0001, 'reg__regressor__batch_size': 32, 'reg__regressor__hidden_layer_sizes': (128, 64), 'reg__regressor__learning_rate_init': 0.001, 'reg__regressor__solver': 'adam'}

Running with seed: 955
R² on test set (log/transformed scale): 0.7412
R² on training set (original scale): 0.9275
R² on test set (original scale): 0.9547
Test MSE: 120872.77
Test MAE: 233.01
Test MAPE (%): 53.68
Best Parameters: {'reg__regressor__activation': 'relu', 'reg__regressor__alpha': 0.0001, 'reg__regressor__batch_size': 32, 'reg__regressor__hidden_layer_sizes': (256, 128, 64), 'reg__regressor__learning_rate_init': 0.0005, 'reg__regressor__solver': 'adam'}

Average Test R² (original scale): 0.8462 ± 0.1534
Average Test R² (log scale): 0.5212 ± 0.3111
Average Test MSE: 410027.18 ± 408926.08
Average Test MAE: 330.47 ± 137.83
Average Test MAPE (%): 121.01 ± 95.23