Case_Study

1. Setup and Data Loading

First, we load all the necessary R packages for data manipulation, modeling, and visualization. We also set some global options for the code chunks.

```
# Load necessary libraries
library(tidyverse)    # For data manipulation and visualization
library(moments)      # For moment calculations
library(car)          # For VIF calculation in linear models
library(mgcv)         # For Generalized Additive Models (GAMs)
library(randomForest) # For Random Forest models
library(kernlab)      # For Gaussian Process models
library(knitr)        # For creating well-formatted tables
library(ggplot2)
library(dplyr)
library(tidyr)
library(tibble)
library(readr)
library(ranger)
library(purrr)
library(patchwork)
library(gratia)

# Set global options for code chunks
knitr::opts_chunk$set(echo = TRUE, message = FALSE, warning = FA
```

1.1. Load Raw Data

We load the training and test datasets provided for the case study. [1, 1]

```
# Load the training and test data
train_raw <- read.csv("data-train.csv")
test_raw <- read.csv("data-test.csv")

# Display the first few rows of the training data
head(train_raw)
```

```
    St  Re    Fr R_moment_1 R_moment_2 R_moment_3 R_moment_4
1 0.10 224 0.052 0.00215700  0.1303500   14.37400  1586.5000
2 3.00 224 0.052 0.00379030  0.4704200   69.94000 10404.0000
3 0.70 224   Inf 0.00290540  0.0434990    0.82200    15.5510
4 0.05  90   Inf 0.06352800  0.0906530    0.46746     3.2696
5 0.70 398   Inf 0.00036945  0.0062242    0.12649     2.5714
6 2.00  90 0.300 0.14780000  2.0068000   36.24900   671.6700
```

2. Data Preparation and Feature Engineering

This section covers the transformation of the raw simulation output into a format suitable for modeling.

2.1. Moment Conversion

The raw data provides the first four raw moments of the particle cluster volume distribution. We need to convert these into the more interpretable summary statistics: mean, standard deviation, skewness, and kurtosis. We create a function to handle this conversion.

```r
## ---- moment-conversion-fixed, message=FALSE, warning=FALSE --

# Safer conversion of raw moments → mean, sd, skewness, kurtosis
calculate_summary_stats <- function(raw_df, eps = 1e-8, return_

  # Check for required columns
  required_cols <- c("R_moment_1", "R_moment_2", "R_moment_3", "
  if (!all(required_cols %in% names(raw_df))) {
    stop("Input must contain columns: R_moment_1–R_moment_4")
  }

  n <- nrow(raw_df)

  # Build raw moment matrix (rows = moment order)
  raw_mat <- rbind(
    rep(1, n),              # 0th raw moment
    raw_df$R_moment_1,      # 1st
    raw_df$R_moment_2,      # 2nd
    raw_df$R_moment_3,      # 3rd
    raw_df$R_moment_4       # 4th
  )
```

```
  # Convert to central moments
  central_mat <- raw2central(raw_mat)

  # Extract central moments
  mu   <- raw_df$R_moment_1
  mu2  <- central_mat[3, ]  # variance
  mu3  <- central_mat[4, ]
  mu4  <- central_mat[5, ]

  # Clean numerical artifacts
  mu2_clean <- pmax(mu2, 0)
  sigma     <- sqrt(mu2_clean)
  sigma_safe <- ifelse(sigma < eps, NA_real_, sigma)

  # Initialize
  gamma <- rep(NA_real_, n)
  kappa <- rep(NA_real_, n)

  # Compute skewness/kurtosis where safe
  valid <- which(!is.na(sigma_safe))
  if (length(valid) > 0) {
    gamma[valid] <- mu3[valid] / (sigma_safe[valid]^3)
    kappa[valid] <- mu4[valid] / (sigma_safe[valid]^4)
  }

  # Optionally flag bad rows
  if (return_flags) {
    flags <- data.frame(
      zero_variance = is.na(sigma_safe),
      negative_mu2  = mu2 < 0
    )
    return(list(summary = data.frame(mu, sigma, gamma, kappa),
  }

  data.frame(mu, sigma, gamma, kappa)
}

# Apply to training data
train_responses <- calculate_summary_stats(train_raw)

# Combine predictors and responses
train_processed <- cbind(train_raw, train_responses)
head(train_processed)
```

```
    St  Re    Fr R_moment_1 R_moment_2 R_moment_3 R_moment_4
mu
1 0.10 224 0.052 0.00215700  0.1303500   14.37400  1586.5000
0.00215700
2 3.00 224 0.052 0.00379030  0.4704200   69.94000 10404.0000
0.00379030
3 0.70 224   Inf 0.00290540  0.0434990    0.82200    15.5510
0.00290540
4 0.05  90   Inf 0.06352800  0.0906530    0.46746     3.2696
0.06352800
5 0.70 398   Inf 0.00036945  0.0062242    0.12649     2.5714
0.00036945
6 2.00  90 0.300 0.14780000  2.0068000   36.24900   671.6700
0.14780000
       sigma     gamma      kappa
1 0.36103372 305.42800 93371.6556
2 0.68586123 216.76225 47012.2515
3 0.20854390  90.58974  8216.7778
4 0.29430799  17.67980   420.2523
5 0.07889273 257.58554 66372.7845
6 1.40888437  12.64607   165.0999
```

2.2.1 Feature Engineering and Transformation

Based on the exploratory analysis, we engineer the `Fr` variable and apply a log transformation to the highly skewed response variables and predictor variable St.

```
## ---- feature-engineering-fixed, message=FALSE, warning=FALSE

# Feature engineering and safe inverse and log transforms
process_features <- function(df) {
  df %>%
    mutate(
      is_gravity_present = ifelse(is.infinite(Fr), 0, 1),
      inv_Fr             = ifelse(is.infinite(Fr), 0, 1 / Fr),
      log_St             = ifelse(St > 0, log(St), NA_real_)
    ) %>%
    select(St, log_St, Re, is_gravity_present, inv_Fr)
}

train_predictors_transformed <- process_features(train_raw)
test_predictors  <- process_features(test_raw)
```

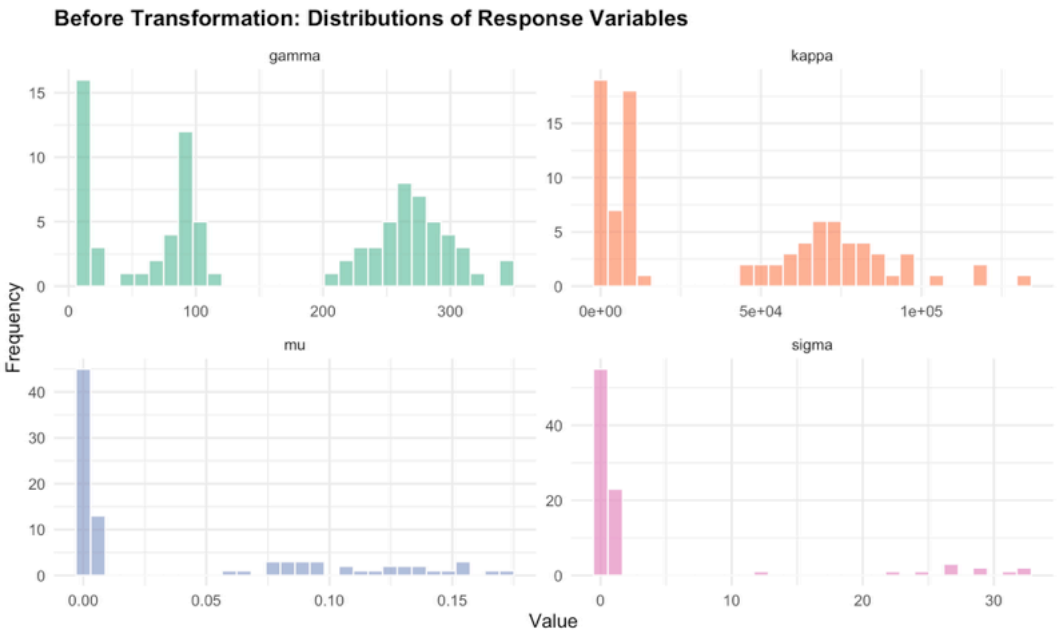
```r
# Safe log transformation for response variables
safe_log_transform <- function(df, small = 1e-8) {
  df %>%
    mutate(
      log_mu     = ifelse(mu     > 0, log(mu),     NA_real_),
      log_sigma  = ifelse(sigma  > 0, log(sigma),  NA_real_),
      log_gamma  = ifelse(gamma  > 0, log(gamma),  NA_real_),
      log_kappa  = ifelse(kappa  > 0, log(kappa),  NA_real_)
    ) %>%
    select(log_mu, log_sigma, log_gamma, log_kappa)
}

train_responses_transformed <- safe_log_transform(train_response


train_final <- cbind(train_predictors_transformed, train_respons

# Identify any problematic (NA or Inf) rows
problem_rows <- which(!is.finite(train_final$log_mu) |
                      !is.finite(train_final$log_sigma) |
                      !is.finite(train_final$log_gamma) |
                      !is.finite(train_final$log_kappa))


head(train_final)
```

```
    St     log_St  Re is_gravity_present    inv_Fr    log_mu
log_sigma
1 0.10 -2.3025851 224                  1 19.230769 -6.139037
-1.0187839
2 3.00  1.0986123 224                  1 19.230769 -5.575310
-0.3770800
3 0.70 -0.3566749 224                  0  0.000000 -5.841184
-1.5676057
4 0.05 -2.9957323  90                  0  0.000000 -2.756275
-1.2231285
5 0.70 -0.3566749 398                  0  0.000000 -7.903495
-2.5396661
6 2.00  0.6931472  90                  1  3.333333 -1.911895
0.3427982
  log_gamma log_kappa
1  5.721714 11.444343
2  5.378801 10.758164
```

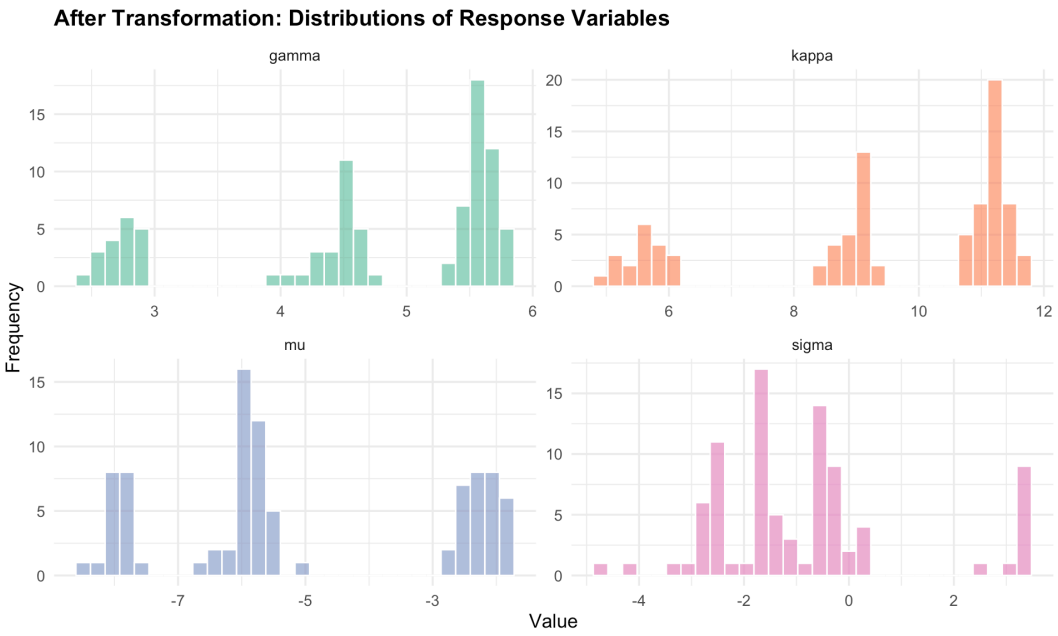
```
3  4.506341  9.013933
4  2.872423  6.040855
5  5.551352 11.103042
6  2.537346  5.106550
```

2.2.2 Univariate EDA of Responses for Current and Transformation

```
## ---- two-faceted-plots, fig.width=10, fig.height=8, message=F

# Prepare separate before and after datasets
before_df <- train_responses %>%
  mutate(stage = "Before Transformation") %>%
  select(stage, mu, sigma, gamma, kappa) %>%
  pivot_longer(cols = c(mu, sigma, gamma, kappa),
               names_to = "variable", values_to = "value")

after_df <- train_final %>%
  mutate(stage = "After Transformation") %>%
  rename(mu = log_mu, sigma = log_sigma, gamma = log_gamma, kapp
  select(stage, mu, sigma, gamma, kappa) %>%
  pivot_longer(cols = c(mu, sigma, gamma, kappa),
               names_to = "variable", values_to = "value")

# --- BEFORE TRANSFORMATION ---
ggplot(before_df, aes(x = value, fill = variable)) +
  geom_histogram(bins = 30, alpha = 0.7, position = "identity",
  facet_wrap(~ variable, scales = "free", ncol = 2) +
  theme_minimal(base_size = 13) +
  scale_fill_brewer(palette = "Set2") +
  labs(
    title = "Before Transformation: Distributions of Response Va
    x = "Value", y = "Frequency"
  ) +
  theme(plot.title = element_text(face = "bold", size = 15),
        legend.position = "none")
```

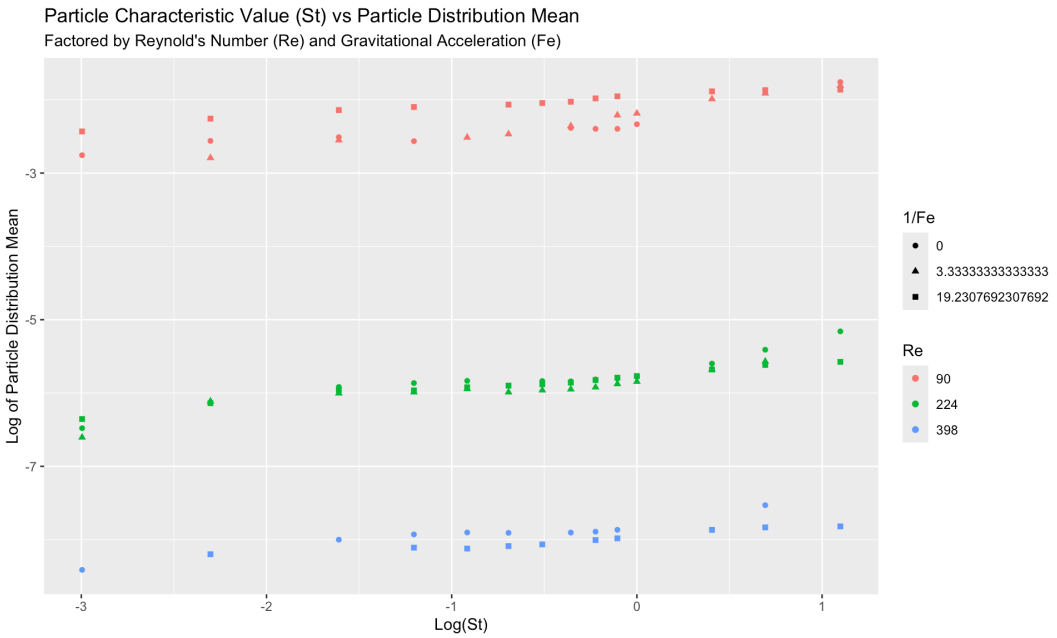



```
# --- AFTER TRANSFORMATION ---
ggplot(after_df, aes(x = value, fill = variable)) +
  geom_histogram(bins = 30, alpha = 0.7, position = "identity",
  facet_wrap(~ variable, scales = "free", ncol = 2) +
  theme_minimal(base_size = 13) +
  scale_fill_brewer(palette = "Set2") +
  labs(
    title = "After Transformation: Distributions of Response Va
    x = "Value", y = "Frequency"
  ) +
  theme(plot.title = element_text(face = "bold", size = 15),
        legend.position = "none")
```

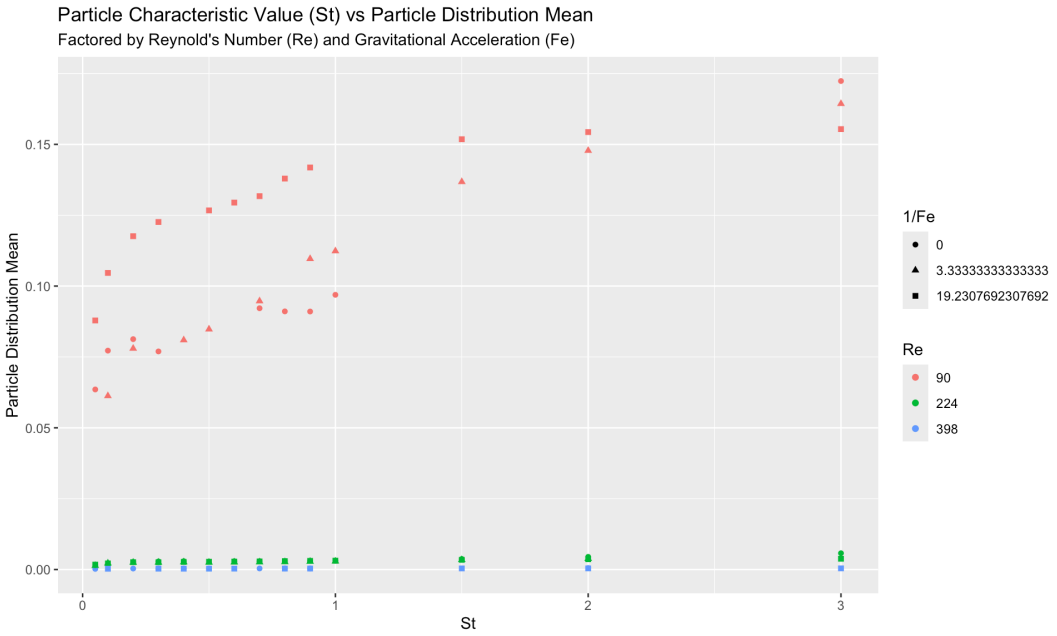


2.2.3 Bivariate EDA of Responses for Current and Transformation

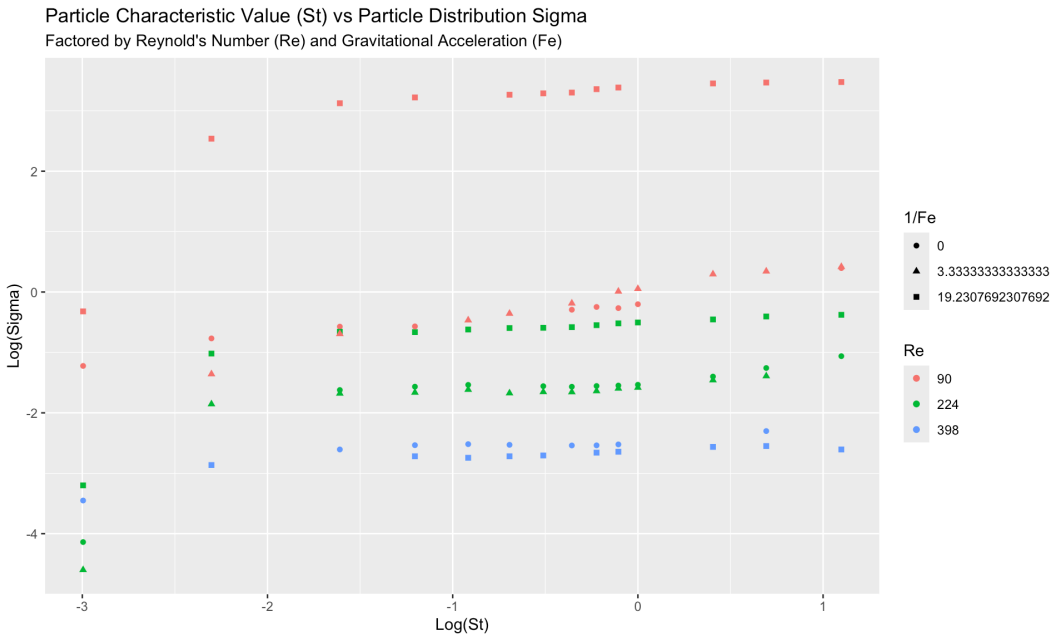
```
ggplot(train_final, aes(x = log_St, y = log_mu, color = factor(R
  geom_point() +
  labs(x = "Log(St)",
       y = "Log of Particle Distribution Mean",
       color = "Re",
       shape = "1/Fe",
       title = "Particle Characteristic Value (St) vs Particle D
       subtitle = "Factored by Reynold's Number (Re) and Gravita
```



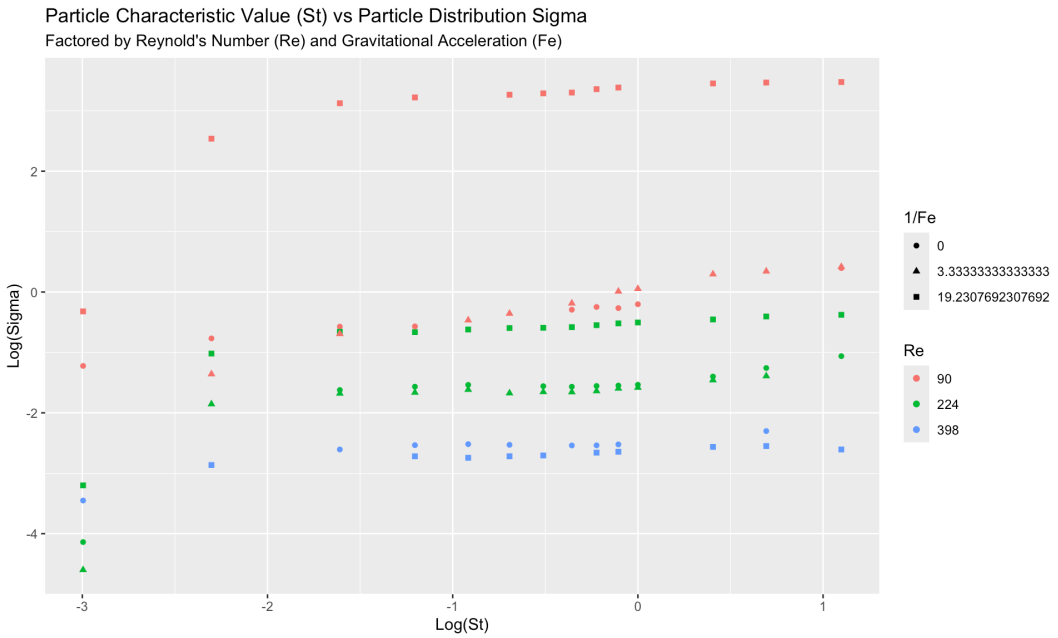

```
ggplot(train_final, aes(x = St, y = exp(log_mu), color = factor
  geom_point() +
  labs(x = "St",
       y = "Particle Distribution Mean",
       color = "Re",
       shape = "1/Fe",
       title = "Particle Characteristic Value (St) vs Particle D
       subtitle = "Factored by Reynold's Number (Re) and Gravita
```



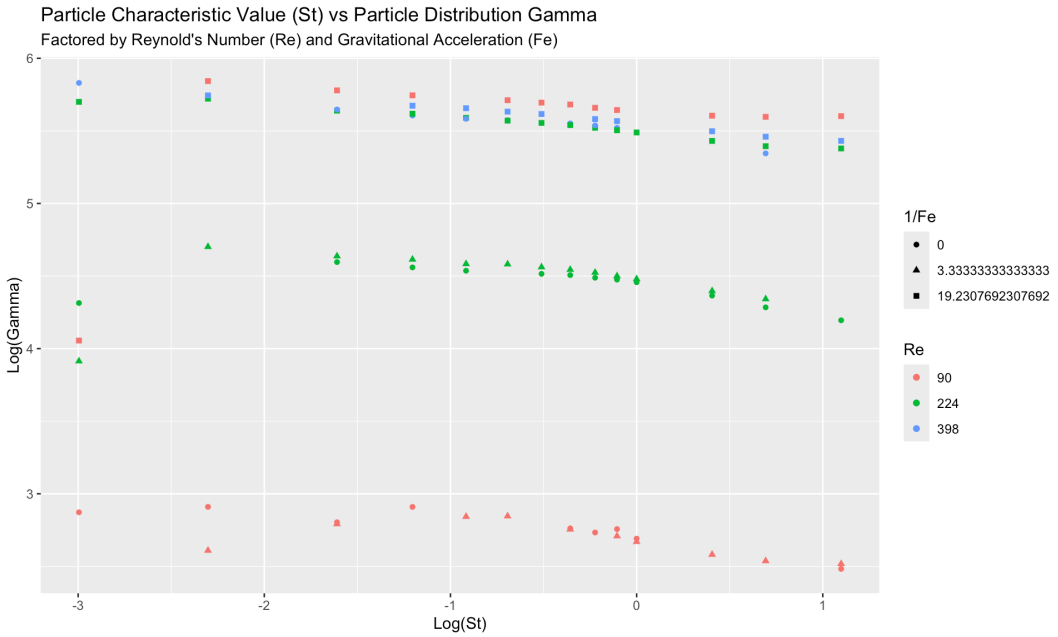
```
ggplot(train_final, aes(x = log_St, y = log_sigma, color = facto
  geom_point() +
  labs(x = "Log(St)",
       y = "Log(Sigma)",
       color = "Re",
       shape = "1/Fe",
       title = "Particle Characteristic Value (St) vs Particle D
       subtitle = "Factored by Reynold's Number (Re) and Gravita
```



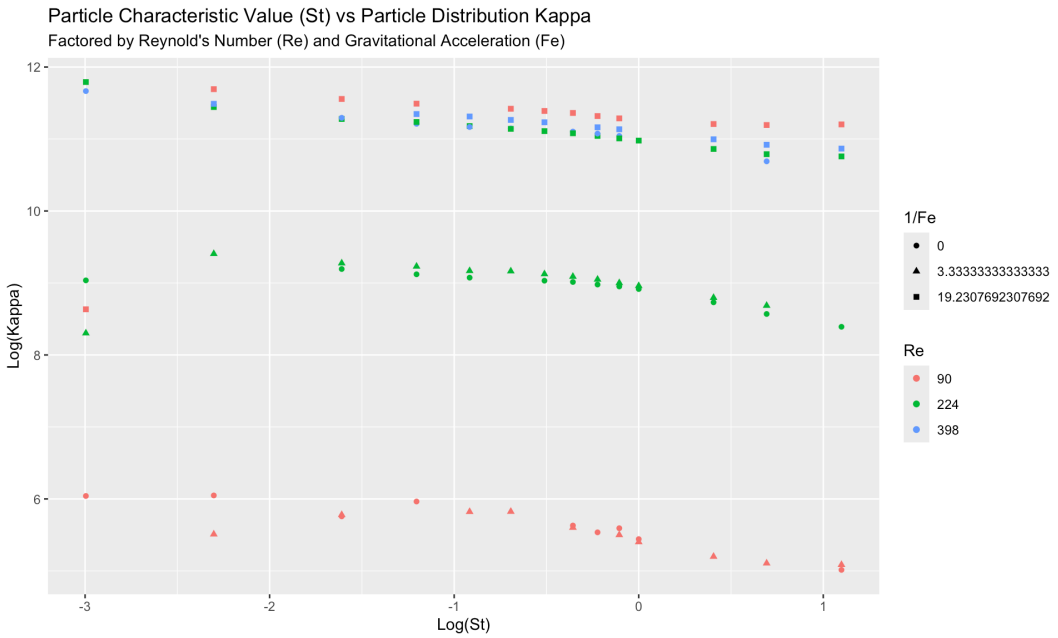

```
ggplot(train_final, aes(x = log_St, y = log_sigma, color = facto
  geom_point() +
  labs(x = "Log(St)",
       y = "Log(Sigma)",
       color = "Re",
       shape = "1/Fe",
       title = "Particle Characteristic Value (St) vs Particle D
       subtitle = "Factored by Reynold's Number (Re) and Gravita
```




```
ggplot(train_final, aes(x = log_St, y = log_gamma, color = facto
  geom_point() +
  labs(x = "Log(St)",
       y = "Log(Gamma)",
       color = "Re",
       shape = "1/Fe",
       title = "Particle Characteristic Value (St) vs Particle D
       subtitle = "Factored by Reynold's Number (Re) and Gravita
```



```
ggplot(train_final, aes(x = log_St, y = log_kappa, color = facto
  geom_point() +
  labs(x = "Log(St)",
       y = "Log(Kappa)",
       color = "Re",
       shape = "1/Fe",
       title = "Particle Characteristic Value (St) vs Particle D
       subtitle = "Factored by Reynold's Number (Re) and Gravita
```



2.3. Exploratory Data Analysis (EDA)

A summary of the final processed data, similar to Table 1 in the report.

```
# Generate descriptive statistics for the final dataset
summary_table <- summary(train_final)

# Print the summary
print(summary_table)
```

```
       St              log_St              Re
is_gravity_present
 Min.   :0.0500   Min.   :-2.9957   Min.   : 90.0   Min.
:0.0000
 1st Qu.:0.3000   1st Qu.:-1.2040   1st Qu.: 90.0   1st
Qu.:0.0000
```

```
 Median :0.7000   Median :-0.3567   Median :224.0   Median
:1.0000
 Mean   :0.8596   Mean   :-0.6148   Mean   :214.5   Mean
:0.6629
 3rd Qu.:1.0000   3rd Qu.: 0.0000   3rd Qu.:224.0   3rd
Qu.:1.0000
 Max.   :3.0000   Max.   : 1.0986   Max.   :398.0   Max.
:1.0000
     inv_Fr           log_mu          log_sigma
log_gamma
 Min.   : 0.000   Min.   :-8.413   Min.   :-4.5992   Min.
:2.483
 1st Qu.: 0.000   1st Qu.:-6.139   1st Qu.:-1.8552   1st
Qu.:4.284
 Median : 3.333   Median :-5.823   Median :-1.2580   Median
:4.702
 Mean   : 8.640   Mean   :-5.051   Mean   :-0.8494   Mean
:4.649
 3rd Qu.:19.231   3rd Qu.:-2.432   3rd Qu.:-0.3205   3rd
Qu.:5.597
 Max.   :19.231   Max.   :-1.758   Max.   : 3.4755   Max.
:5.843
   log_kappa
 Min.   : 5.014
 1st Qu.: 8.635
 Median : 9.406
 Mean   : 9.345
 3rd Qu.:11.195
 Max.   :11.792
```

3. Linear Fitting

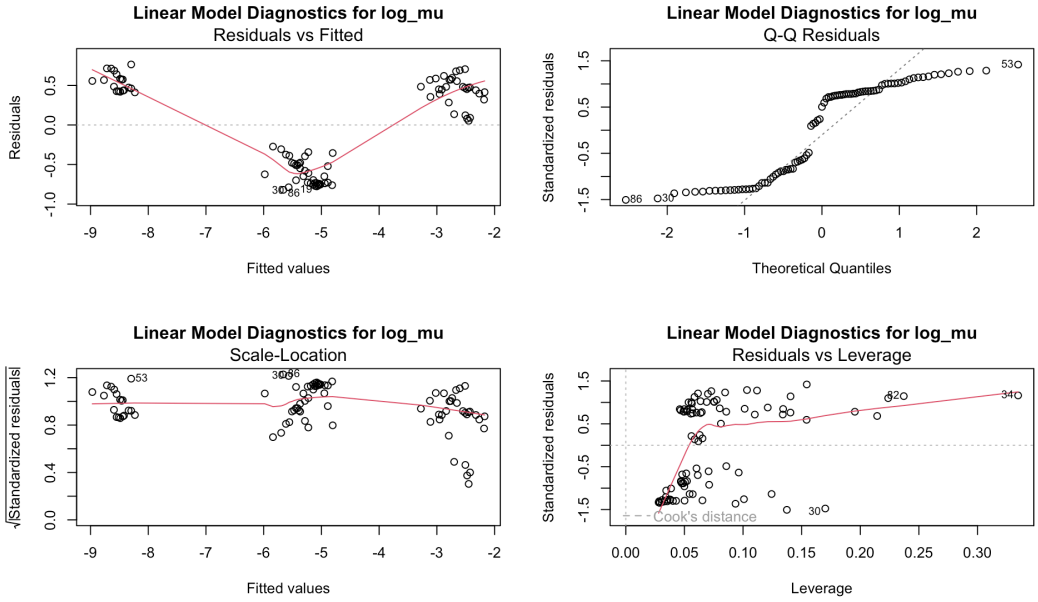
We establish a baseline by fitting a linear model. This helps formally test for non-linearity.

```
## 3. Baseline Model: Multivariate Linear Regression
# Define a list of response variables
responses <- c("log_mu", "log_sigma", "log_gamma", "log_kappa")
lm_models <- list()
lm_rmse <- list()

# Loop through each response to build a model
for (response in responses) {
  formula_str <- paste(response, "~ log_St * Re + log_St * inv_
```

```
  model <- lm(as.formula(formula_str), data = train_final)
  lm_models[[response]] <- model

  # Print model summary
  cat("--- Linear Model Summary for", response, "---\n")
  print(summary(model))
  summary(model)

  # Diagnostic plots
  par(mfrow = c(2, 2))
  plot(model, main = paste("Linear Model Diagnostics for", respo
  par(mfrow = c(1, 1))

  # Check for multicollinearity
  cat("\n--- VIF for", response, "---\n")
  print(vif(model))

  # Predict on test set and calculate RMSE
  predictions <- predict(model, newdata = test_predictors)
  # Note: We don't have true values for the test set, so RMSE is
  train_preds <- predict(model, newdata = train_final)
  rmse <- sqrt(mean((train_final[[response]] - train_preds)^2))
  lm_rmse[[response]] <- rmse
  cat("\nTraining RMSE for", response, ":", rmse, "\n\n")
}
```

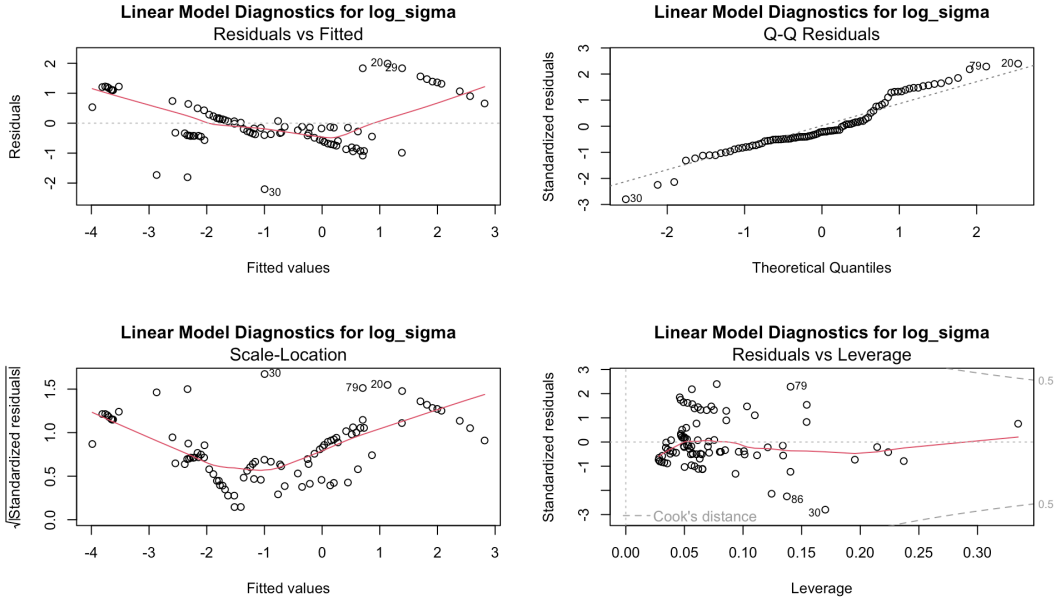
```
--- Linear Model Summary for log_mu ---

Call:
lm(formula = as.formula(formula_str), data = train_final)

Residuals:
    Min      1Q  Median      3Q     Max
-0.8202 -0.6086  0.2837  0.4825  0.7651

Coefficients:
                    Estimate Std. Error t value Pr(>|t|)
(Intercept)       -0.6721985  0.1910452  -3.519 0.000711 ***
log_St             0.2428634  0.1329873   1.826 0.071457 .
Re                -0.0194721  0.0006616 -29.434  < 2e-16 ***
inv_Fr             0.0221405  0.0108734   2.036 0.044958 *
is_gravity_present -0.4079125  0.1900942  -2.146 0.034842 *
log_St:Re         -0.0001516  0.0005290  -0.287 0.775215
log_St:inv_Fr     -0.0012936  0.0065406  -0.198 0.843702
```

```
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.5862 on 82 degrees of freedom
Multiple R-squared:  0.9361,    Adjusted R-squared:  0.9314
F-statistic: 200.2 on 6 and 82 DF,  p-value: < 2.2e-16
```



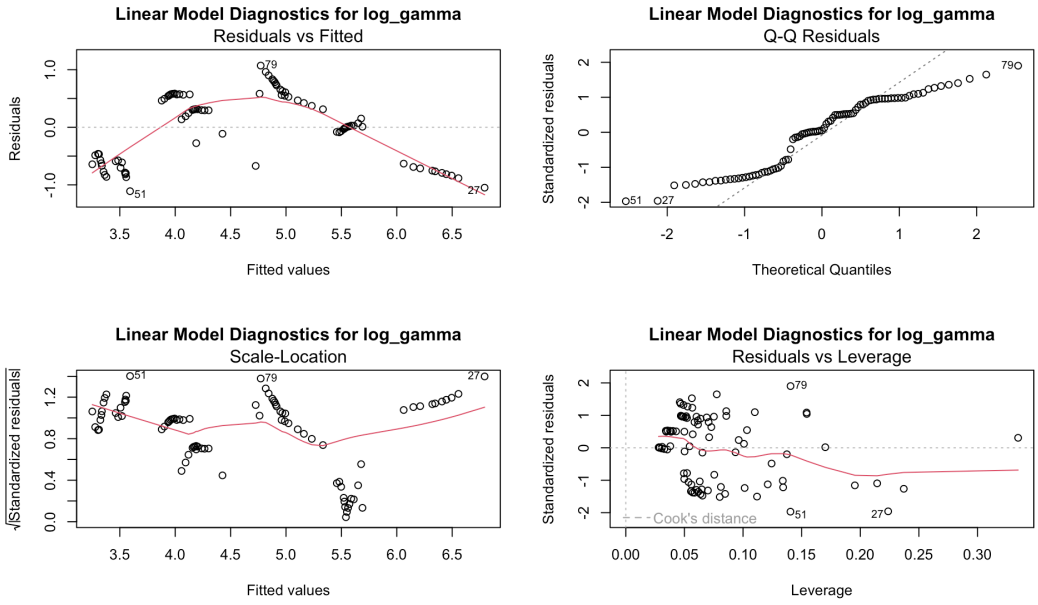

```
--- VIF for log_mu ---

            log_St                 Re             inv_Fr
is_gravity_present
          5.271437           1.431111           2.382366
2.091076
         log_St:Re      log_St:inv_Fr
          4.768897           2.231717

Training RMSE for log_mu : 0.5627138

--- Linear Model Summary for log_sigma ---

Call:
lm(formula = as.formula(formula_str), data = train_final)

Residuals:
    Min      1Q  Median      3Q     Max
-2.2036 -0.4472 -0.1774  0.4958  1.9892
```

```
Coefficients:
                   Estimate Std. Error t value Pr(>|t|)
(Intercept)         1.9945869  0.2816818   7.081 4.47e-10 ***
log_St              0.7353162  0.1960798   3.750 0.000328 ***
Re                 -0.0140829  0.0009754 -14.438  < 2e-16 ***
inv_Fr              0.1214802  0.0160321   7.577 4.77e-11 ***
is_gravity_present -0.9280740  0.2802796  -3.311 0.001383 **
log_St:Re          -0.0015341  0.0007800  -1.967 0.052593 .
log_St:inv_Fr       0.0012419  0.0096436   0.129 0.897846
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.8644 on 82 degrees of freedom
Multiple R-squared:  0.7979,    Adjusted R-squared:  0.7831
F-statistic: 53.95 on 6 and 82 DF,  p-value: < 2.2e-16
```



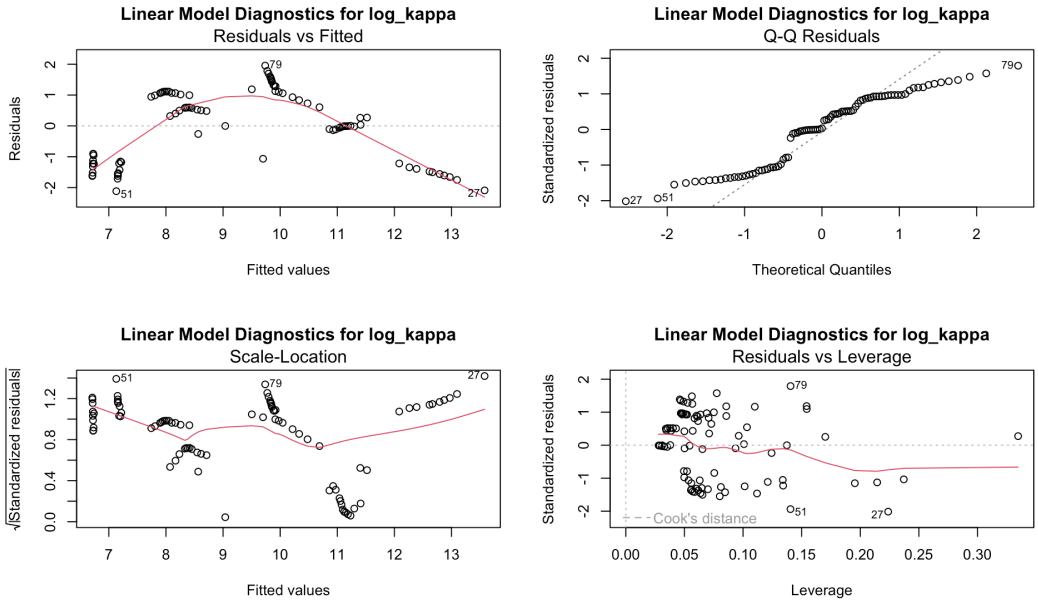

```
--- VIF for log_sigma ---

           log_St                Re            inv_Fr
is_gravity_present
         5.271437          1.431111          2.382366
2.091076
        log_St:Re      log_St:inv_Fr
         4.768897          2.231717

Training RMSE for log_sigma : 0.8296791
```

```
--- Linear Model Summary for log_gamma ---

Call:
lm(formula = as.formula(formula_str), data = train_final)

Residuals:
    Min      1Q  Median      3Q     Max
-1.1095 -0.6250  0.0293  0.5485  1.0717

Coefficients:
                   Estimate Std. Error t value Pr(>|t|)
(Intercept)        3.1552562  0.1980162  15.934  < 2e-16 ***
log_St             0.1134506  0.1378398   0.823  0.41286
Re                 0.0044685  0.0006857   6.517 5.46e-09 ***
inv_Fr             0.0996511  0.0112702   8.842 1.48e-13 ***
is_gravity_present -0.5518587  0.1970305  -2.801  0.00635 **
log_St:Re          -0.0009094  0.0005483  -1.658  0.10105
log_St:inv_Fr       0.0017522  0.0067793   0.258  0.79670
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.6076 on 82 degrees of freedom
Multiple R-squared:  0.731, Adjusted R-squared:  0.7113
F-statistic: 37.14 on 6 and 82 DF,  p-value: < 2.2e-16
```




```
--- VIF for log_gamma ---
```

```
            log_St                  Re             inv_Fr
is_gravity_present
          5.271437           1.431111           2.382366
2.091076
         log_St:Re      log_St:inv_Fr
          4.768897           2.231717

Training RMSE for log_gamma : 0.5832464

--- Linear Model Summary for log_kappa ---

Call:
lm(formula = as.formula(formula_str), data = train_final)

Residuals:
     Min       1Q   Median       3Q      Max
-2.11612 -1.21534  0.03521  1.05915  1.95539

Coefficients:
                   Estimate Std. Error t value Pr(>|t|)
(Intercept)         6.362896   0.383797  16.579  < 2e-16 ***
log_St              0.122808   0.267162   0.460  0.64697
Re                  0.008787   0.001329   6.612 3.59e-09 ***
inv_Fr              0.197611   0.021844   9.046 5.82e-14 ***
is_gravity_present -1.092790   0.381886  -2.862  0.00535 **
log_St:Re          -0.001602   0.001063  -1.507  0.13560
log_St:inv_Fr       0.003907   0.013140   0.297  0.76698
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 1.178 on 82 degrees of freedom
Multiple R-squared:  0.737, Adjusted R-squared:  0.7178
F-statistic: 38.31 on 6 and 82 DF,  p-value: < 2.2e-16
```




```
--- VIF for log_kappa ---

            log_St                 Re             inv_Fr
is_gravity_present
          5.271437           1.431111           2.382366
2.091076
         log_St:Re      log_St:inv_Fr
          4.768897           2.231717

Training RMSE for log_kappa : 1.130454
```

1. Model for log_mu and log_sigma (First & Second Images)

For the models predicting the log-transformed mean and standard deviation, the diagnostic plots reveal several significant issues:

Failure of Linearity Assumption: The Residuals vs. Fitted plots for both models show a distinct, curvilinear pattern in the residuals. The smoothed red line follows a clear U-shape rather than being flat and straight. This is a classic sign that the linear model is failing to capture the true underlying non-linear relationships in the data. It is systematically mis-predicting in different regions of the data.

Non-Normal Residuals: The Normal Q-Q plots show that the residuals deviate from the theoretical diagonal line, particularly at the tails. This indicates that the errors of the model are not normally distributed;

specifically, they have heavier tails than a normal distribution would suggest, violating a key assumption of linear regression.

Non-Constant Variance (Heteroscedasticity): In the Scale-Location plot, especially for log_sigma, the smoothed line is not flat. It trends upwards, indicating that the variance of the residuals increases as the fitted (predicted) value gets larger. This means the model's predictions are less reliable for larger-scale outcomes.

Presence of Influential Points: The Residuals vs. Leverage plots highlight that some data points have high leverage or large residuals. These points have an unusually strong influence on the estimated coefficients of the model, potentially making the fit unstable and sensitive to a small subset of the data.

Conclusion: For log_mu and log_sigma, the linear model is inadequate as it violates the core assumptions of linearity, normality of residuals, and constant variance.

2. Model for gamma (Skewness - Third Image)

The diagnostics for the gamma model are even more problematic:

Dominance by an Extreme Outlier: All four diagnostic plots are dominated by a single, extreme point with a very large residual.

Severe Violation of Normality: The Normal Q-Q plot shows a catastrophic failure of the normality assumption. One point lies so far from the diagonal line that it renders the plot almost unreadable for the other points, indicating the model is completely unable to account for this observation.

Extreme Influence: The Residuals vs. Leverage plot confirms that this outlier is an extremely influential point, falling far outside the standard contours of Cook's distance. This means this single data point is fundamentally distorting the entire model fit.

Conclusion: The linear model for gamma is invalid. It is not robust and its results are unreliable due to the overwhelming effect of at least one influential outlier.

3. Model for log_kappa (Kurtosis - Fourth Image)

The diagnostics for log_kappa mirror the issues seen with log_mu and log_sigma:

Clear Non-Linearity: The Residuals vs. Fitted plot again shows a pronounced U-shaped pattern, failing the linearity assumption.

Non-Normal Residuals: The Normal Q-Q plot shows points peeling away from the diagonal line at the tails, violating the normality assumption.

Influential Points: The model is again sensitive to a few points with high leverage or large residuals.

Conclusion: The linear model for log_kappa is also a poor fit, failing on the same key assumptions as the other models.

Therefore, we must explore either more complex parametric models or non-linear models.

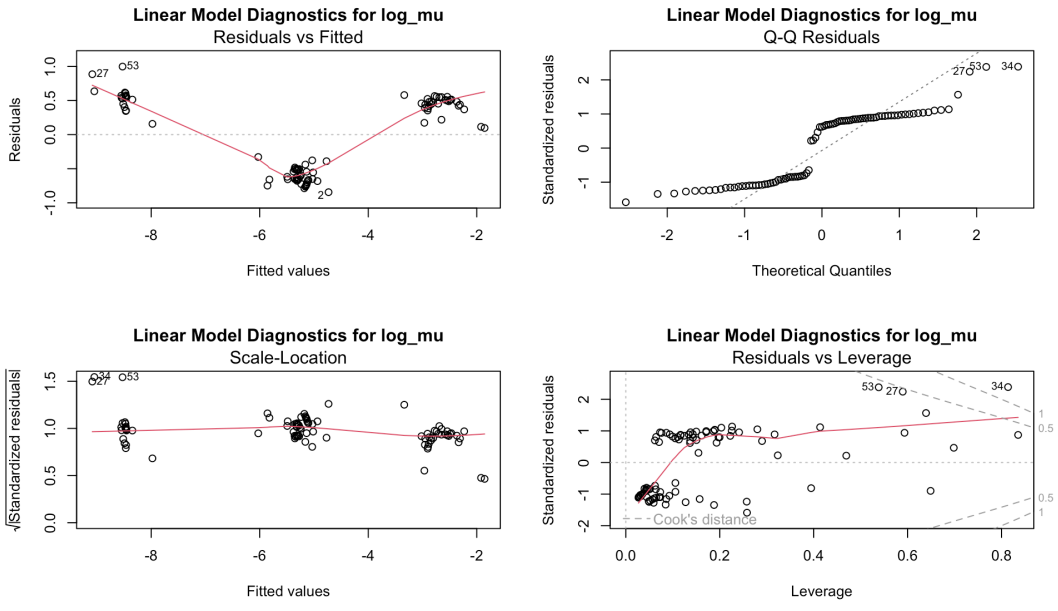
3b. Cubic Modeling

```
cm_models <- list()
cm_rmse <- list()

# Loop through each response to build a model
for (response in responses) {
  formula_str <- paste(response, "~ poly(log_St, 3, raw = TRUE)+
  model <- lm(as.formula(formula_str), data = train_final)
  lm_models[[response]] <- model

  # Print model summary
  cat("--- Linear Model Summary for", response, "---\n")
  print(summary(model))
  summary(model)

  # Diagnostic plots
  par(mfrow = c(2, 2))
  plot(model, main = paste("Linear Model Diagnostics for", respo
  par(mfrow = c(1, 1))

  # Check for multicollinearity
  cat("\n--- VIF for", response, "---\n")
  print(vif(model))

  # Predict on test set and calculate RMSE
  predictions <- predict(model, newdata = test_predictors)
  # Note: We don't have true values for the test set, so RMSE is
  train_preds <- predict(model, newdata = train_final)
```

```
  rmse <- sqrt(mean((train_final[[response]] - train_preds)^2))
  lm_rmse[[response]] <- rmse
  cat("\nTraining RMSE for", response, ":", rmse, "\n\n")
}
```

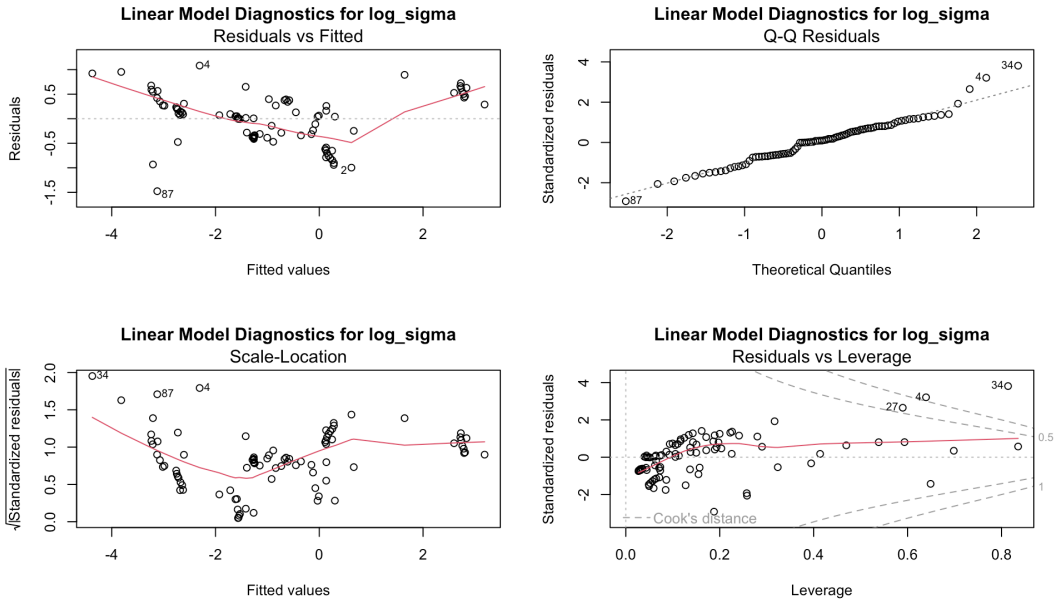
```
--- Linear Model Summary for log_mu ---

Call:
lm(formula = as.formula(formula_str), data = train_final)

Residuals:
    Min      1Q  Median      3Q     Max 
-0.8440 -0.6187  0.3462  0.5095  0.9974 

Coefficients:
                                      Estimate Std. Error t
value Pr(>|t|)
(Intercept)                         -1.144e+00  3.022e-01
-3.786 0.000312
poly(log_St, 3, raw = TRUE)1         5.344e-01  3.370e-01
1.586 0.117127
poly(log_St, 3, raw = TRUE)2         4.314e-01  3.788e-01
1.139 0.258567
poly(log_St, 3, raw = TRUE)3         1.039e-01  1.278e-01
0.813 0.418922
Re                                  -1.843e-02  1.303e-03
-14.146  < 2e-16
inv_Fr                               2.499e-02  2.457e-02
1.017 0.312638
poly(log_St, 3, raw = TRUE)1:Re     -1.497e-03  1.555e-03
-0.963 0.338679
poly(log_St, 3, raw = TRUE)2:Re     -1.149e-03  1.926e-03
-0.597 0.552618
poly(log_St, 3, raw = TRUE)3:Re     -2.124e-04  6.026e-04
-0.353 0.725435
poly(log_St, 3, raw = TRUE)1:inv_Fr -1.502e-02  2.653e-02
-0.566 0.572924
poly(log_St, 3, raw = TRUE)2:inv_Fr -2.586e-02  3.040e-02
-0.851 0.397775
poly(log_St, 3, raw = TRUE)3:inv_Fr -8.514e-03  1.065e-02
-0.800 0.426498
Re:inv_Fr                           -7.225e-05  9.911e-05
-0.729 0.468343
poly(log_St, 3, raw = TRUE)1:Re:inv_Fr  4.957e-05  1.120e-04
```

```
0.443 0.659314
poly(log_St, 3, raw = TRUE)2:Re:inv_Fr  1.044e-04  1.359e-04
0.769 0.444622
poly(log_St, 3, raw = TRUE)3:Re:inv_Fr  3.952e-05  4.802e-05
0.823 0.413185

(Intercept)                             ***
poly(log_St, 3, raw = TRUE)1
poly(log_St, 3, raw = TRUE)2
poly(log_St, 3, raw = TRUE)3
Re                                      ***
inv_Fr
poly(log_St, 3, raw = TRUE)1:Re
poly(log_St, 3, raw = TRUE)2:Re
poly(log_St, 3, raw = TRUE)3:Re
poly(log_St, 3, raw = TRUE)1:inv_Fr
poly(log_St, 3, raw = TRUE)2:inv_Fr
poly(log_St, 3, raw = TRUE)3:inv_Fr
Re:inv_Fr
poly(log_St, 3, raw = TRUE)1:Re:inv_Fr
poly(log_St, 3, raw = TRUE)2:Re:inv_Fr
poly(log_St, 3, raw = TRUE)3:Re:inv_Fr
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.617 on 73 degrees of freedom
Multiple R-squared:  0.937, Adjusted R-squared:  0.924
F-statistic: 72.34 on 15 and 73 DF,  p-value: < 2.2e-16
```



```
--- VIF for log_mu ---

                                             GVIF Df
GVIF^(1/(2*Df))
poly(log_St, 3, raw = TRUE)            728.366174  3
2.999565
Re                                       5.010147  1
2.238336
inv_Fr                                  10.984233  1
3.314247
poly(log_St, 3, raw = TRUE):Re        1166.709494  3
3.244595
poly(log_St, 3, raw = TRUE):inv_Fr    1236.492582  3
3.276161
Re:inv_Fr                               14.545184  1
3.813815
poly(log_St, 3, raw = TRUE):Re:inv_Fr 1702.654477  3
3.455581

Training RMSE for log_mu : 0.5588266

--- Linear Model Summary for log_sigma ---

Call:
lm(formula = as.formula(formula_str), data = train_final)

Residuals:
     Min       1Q   Median       3Q      Max
-1.47666 -0.35223  0.05101  0.37630  1.08276

Coefficients:
                                         Estimate Std. Error t
value Pr(>|t|)
(Intercept)                             6.004e-02  2.749e-01
0.218    0.828
poly(log_St, 3, raw = TRUE)1            4.168e-01  3.066e-01
1.359    0.178
poly(log_St, 3, raw = TRUE)2            1.825e-01  3.447e-01
0.529    0.598
poly(log_St, 3, raw = TRUE)3            7.998e-02  1.163e-01
0.688    0.494
Re                                     -7.093e-03  1.185e-03
-5.984 7.45e-08
```

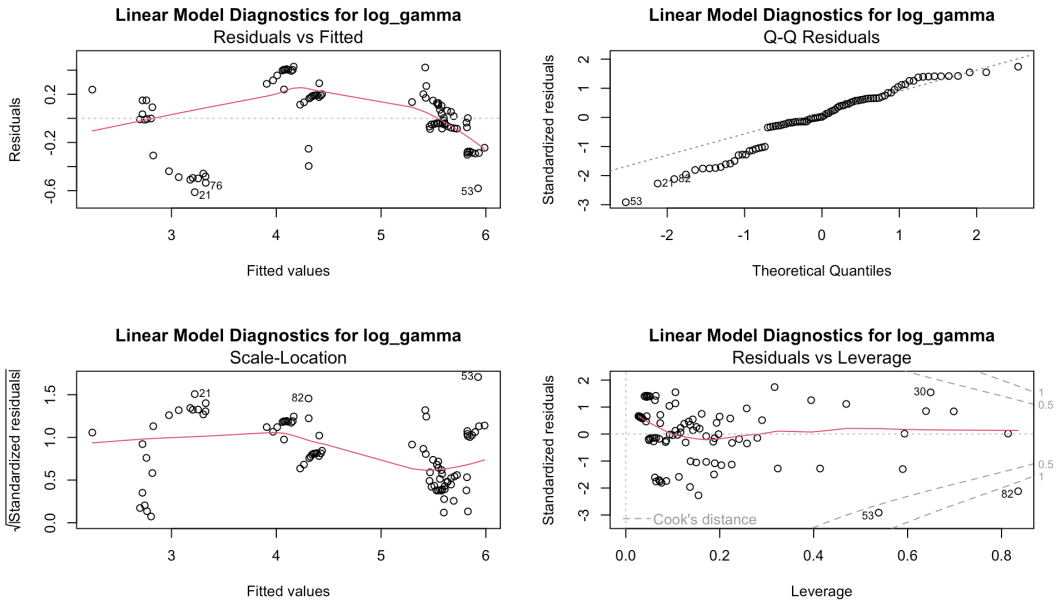
```
inv_Fr                                   2.282e-01  2.236e-02
10.207 1.06e-15
poly(log_St, 3, raw = TRUE)1:Re         -1.105e-03  1.415e-03
-0.781    0.437
poly(log_St, 3, raw = TRUE)2:Re          1.780e-04  1.752e-03
0.102    0.919
poly(log_St, 3, raw = TRUE)3:Re          1.685e-04  5.483e-04
0.307    0.759
poly(log_St, 3, raw = TRUE)1:inv_Fr     -2.492e-02  2.414e-02
-1.033    0.305
poly(log_St, 3, raw = TRUE)2:inv_Fr      1.679e-03  2.766e-02
0.061    0.952
poly(log_St, 3, raw = TRUE)3:inv_Fr      6.453e-03  9.688e-03
0.666    0.507
Re:inv_Fr                               -6.375e-04  9.018e-05
-7.070 7.73e-10
poly(log_St, 3, raw = TRUE)1:Re:inv_Fr   4.786e-05  1.019e-04
0.470    0.640
poly(log_St, 3, raw = TRUE)2:Re:inv_Fr   6.312e-06  1.236e-04
0.051    0.959
poly(log_St, 3, raw = TRUE)3:Re:inv_Fr -7.099e-06  4.369e-05
-0.162    0.871

(Intercept)
poly(log_St, 3, raw = TRUE)1
poly(log_St, 3, raw = TRUE)2
poly(log_St, 3, raw = TRUE)3
Re                                      ***
inv_Fr                                  ***
poly(log_St, 3, raw = TRUE)1:Re
poly(log_St, 3, raw = TRUE)2:Re
poly(log_St, 3, raw = TRUE)3:Re
poly(log_St, 3, raw = TRUE)1:inv_Fr
poly(log_St, 3, raw = TRUE)2:inv_Fr
poly(log_St, 3, raw = TRUE)3:inv_Fr
Re:inv_Fr                               ***
poly(log_St, 3, raw = TRUE)1:Re:inv_Fr
poly(log_St, 3, raw = TRUE)2:Re:inv_Fr
poly(log_St, 3, raw = TRUE)3:Re:inv_Fr
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.5614 on 73 degrees of freedom
Multiple R-squared:  0.9241,    Adjusted R-squared:  0.9085
F-statistic: 59.24 on 15 and 73 DF,  p-value: < 2.2e-16
```




```
--- VIF for log_sigma ---

                                              GVIF Df
GVIF^(1/(2*Df))
poly(log_St, 3, raw = TRUE)            728.366174  3
2.999565
Re                                       5.010147  1
2.238336
inv_Fr                                  10.984233  1
3.314247
poly(log_St, 3, raw = TRUE):Re        1166.709494  3
3.244595
poly(log_St, 3, raw = TRUE):inv_Fr    1236.492582  3
3.276161
Re:inv_Fr                               14.545184  1
3.813815
poly(log_St, 3, raw = TRUE):Re:inv_Fr 1702.654477  3
3.455581

Training RMSE for log_sigma : 0.5084525

--- Linear Model Summary for log_gamma ---

Call:
lm(formula = as.formula(formula_str), data = train_final)

Residuals:
```

```
     Min       1Q   Median       3Q      Max 
-0.61253 -0.08548  0.00266  0.18352  0.42969 

Coefficients:
                                        Estimate Std. Error t
value Pr(>|t|)
(Intercept)                             1.786e+00  1.437e-01
12.429   <2e-16
poly(log_St, 3, raw = TRUE)1           -3.151e-01  1.602e-01
-1.966   0.0531
poly(log_St, 3, raw = TRUE)2           -2.171e-01  1.801e-01
-1.206   0.2319
poly(log_St, 3, raw = TRUE)3           -3.849e-02  6.077e-02
-0.633   0.5284
Re                                      1.015e-02  6.194e-04
16.390   <2e-16
inv_Fr                                  1.892e-01  1.168e-02
16.197   <2e-16
poly(log_St, 3, raw = TRUE)1:Re         8.867e-04  7.391e-04
1.200   0.2341
poly(log_St, 3, raw = TRUE)2:Re         8.625e-04  9.156e-04
0.942   0.3493
poly(log_St, 3, raw = TRUE)3:Re         1.917e-04  2.865e-04
0.669   0.5055
poly(log_St, 3, raw = TRUE)1:inv_Fr    -1.089e-03  1.261e-02
-0.086   0.9314
poly(log_St, 3, raw = TRUE)2:inv_Fr     2.674e-02  1.445e-02
1.850   0.0684
poly(log_St, 3, raw = TRUE)3:inv_Fr     1.272e-02  5.062e-03
2.514   0.0142
Re:inv_Fr                              -5.036e-04  4.712e-05
-10.687   <2e-16
poly(log_St, 3, raw = TRUE)1:Re:inv_Fr -8.851e-07  5.324e-05
-0.017   0.9868
poly(log_St, 3, raw = TRUE)2:Re:inv_Fr -1.044e-04  6.460e-05
-1.616   0.1105
poly(log_St, 3, raw = TRUE)3:Re:inv_Fr -5.019e-05  2.283e-05
-2.199   0.0311

(Intercept)                            ***
poly(log_St, 3, raw = TRUE)1           .
poly(log_St, 3, raw = TRUE)2
poly(log_St, 3, raw = TRUE)3
Re                                     ***
inv_Fr                                 ***
```

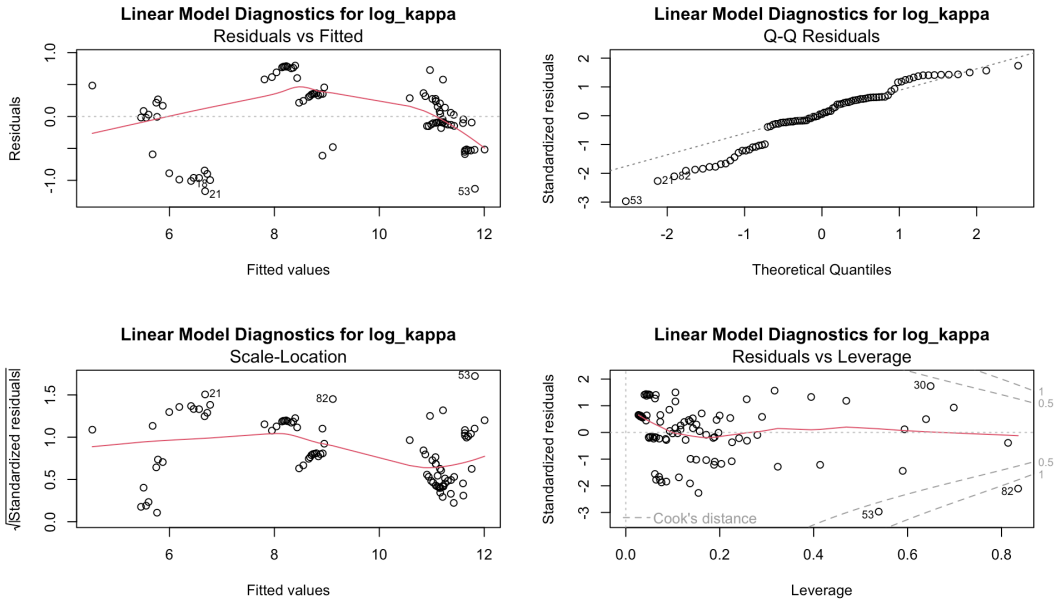
```
poly(log_St, 3, raw = TRUE)1:Re
poly(log_St, 3, raw = TRUE)2:Re
poly(log_St, 3, raw = TRUE)3:Re
poly(log_St, 3, raw = TRUE)1:inv_Fr
poly(log_St, 3, raw = TRUE)2:inv_Fr    .
poly(log_St, 3, raw = TRUE)3:inv_Fr    *
Re:inv_Fr                              ***
poly(log_St, 3, raw = TRUE)1:Re:inv_Fr
poly(log_St, 3, raw = TRUE)2:Re:inv_Fr
poly(log_St, 3, raw = TRUE)3:Re:inv_Fr *
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.2934 on 73 degrees of freedom
Multiple R-squared:  0.9442,    Adjusted R-squared:  0.9327
F-statistic: 82.32 on 15 and 73 DF,  p-value: < 2.2e-16
```




```
--- VIF for log_gamma ---

                                        GVIF Df
GVIF^(1/(2*Df))
poly(log_St, 3, raw = TRUE)         728.366174  3
2.999565
Re                                    5.010147  1
2.238336
inv_Fr                               10.984233  1
3.314247
```

```
poly(log_St, 3, raw = TRUE):Re        1166.709494  3
3.244595
poly(log_St, 3, raw = TRUE):inv_Fr    1236.492582  3
3.276161
Re:inv_Fr                               14.545184  1
3.813815
poly(log_St, 3, raw = TRUE):Re:inv_Fr 1702.654477  3
3.455581

Training RMSE for log_gamma : 0.2656794

--- Linear Model Summary for log_kappa ---

Call:
lm(formula = as.formula(formula_str), data = train_final)

Residuals:
     Min       1Q   Median       3Q      Max
-1.16999 -0.15164  0.02901  0.34292  0.79700

Coefficients:
                                      Estimate Std. Error t
value Pr(>|t|)
(Intercept)                           3.652e+00  2.749e-01
13.285   <2e-16
poly(log_St, 3, raw = TRUE)1         -6.597e-01  3.066e-01
-2.152   0.0347
poly(log_St, 3, raw = TRUE)2         -4.087e-01  3.446e-01
-1.186   0.2394
poly(log_St, 3, raw = TRUE)3         -8.154e-02  1.163e-01
-0.701   0.4854
Re                                    2.007e-02  1.185e-03
16.933   <2e-16
inv_Fr                                3.759e-01  2.235e-02
16.814   <2e-16
poly(log_St, 3, raw = TRUE)1:Re       1.877e-03  1.414e-03
1.327   0.1885
poly(log_St, 3, raw = TRUE)2:Re       1.569e-03  1.752e-03
0.896   0.3733
poly(log_St, 3, raw = TRUE)3:Re       3.501e-04  5.481e-04
0.639   0.5250
poly(log_St, 3, raw = TRUE)1:inv_Fr   2.607e-03  2.413e-02
0.108   0.9142
poly(log_St, 3, raw = TRUE)2:inv_Fr   4.878e-02  2.766e-02
1.764   0.0819
```

```
poly(log_St, 3, raw = TRUE)3:inv_Fr     2.311e-02  9.685e-03
2.386   0.0196
Re:inv_Fr                              -9.977e-04  9.016e-05
-11.066   <2e-16
poly(log_St, 3, raw = TRUE)1:Re:inv_Fr -1.246e-05  1.019e-04
-0.122   0.9030
poly(log_St, 3, raw = TRUE)2:Re:inv_Fr -1.949e-04  1.236e-04
-1.577   0.1191
poly(log_St, 3, raw = TRUE)3:Re:inv_Fr -9.413e-05  4.368e-05
-2.155   0.0345

(Intercept)                            ***
poly(log_St, 3, raw = TRUE)1           *
poly(log_St, 3, raw = TRUE)2
poly(log_St, 3, raw = TRUE)3
Re                                     ***
inv_Fr                                 ***
poly(log_St, 3, raw = TRUE)1:Re
poly(log_St, 3, raw = TRUE)2:Re
poly(log_St, 3, raw = TRUE)3:Re
poly(log_St, 3, raw = TRUE)1:inv_Fr
poly(log_St, 3, raw = TRUE)2:inv_Fr    .
poly(log_St, 3, raw = TRUE)3:inv_Fr    *
Re:inv_Fr                              ***
poly(log_St, 3, raw = TRUE)1:Re:inv_Fr
poly(log_St, 3, raw = TRUE)2:Re:inv_Fr
poly(log_St, 3, raw = TRUE)3:Re:inv_Fr *
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.5613 on 73 degrees of freedom
Multiple R-squared:  0.9468,    Adjusted R-squared:  0.9359
F-statistic: 86.66 on 15 and 73 DF,  p-value: < 2.2e-16
```




```
--- VIF for log_kappa ---

                                              GVIF Df
GVIF^(1/(2*Df))
poly(log_St, 3, raw = TRUE)            728.366174  3
2.999565
Re                                       5.010147  1
2.238336
inv_Fr                                  10.984233  1
3.314247
poly(log_St, 3, raw = TRUE):Re        1166.709494  3
3.244595
poly(log_St, 3, raw = TRUE):inv_Fr    1236.492582  3
3.276161
Re:inv_Fr                               14.545184  1
3.813815
poly(log_St, 3, raw = TRUE):Re:inv_Fr 1702.654477  3
3.455581

Training RMSE for log_kappa : 0.5083405
```

4. Advanced Modeling: Generalized Additive Models (GAMs)

The linear model diagnostics clearly showed that a simple linear relationship is not appropriate. We will now fit a Generalized Additive

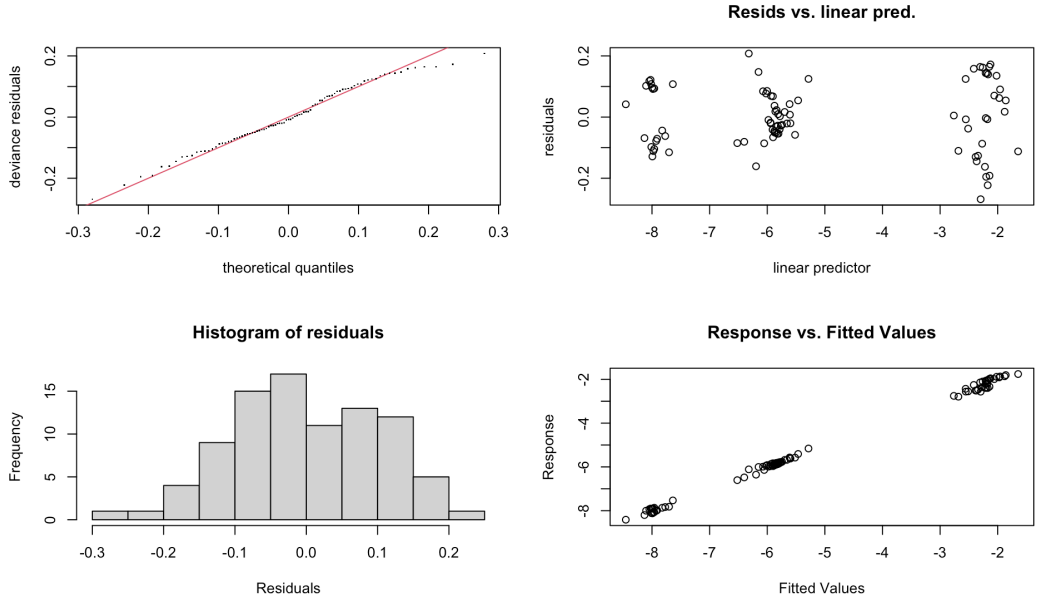
Model (GAM) for each response.

```
# Prepare data for factor modeling
# We use the original 'Re' and 'inv_Fr' and explicitly make ther
train_final_gam <- train_final %>%
  mutate(
    log_St_s = as.numeric(scale(log_St)), # Keep scaled continuc
    Re = factor(Re),               # Treat as a factor
    inv_Fr = factor(round(inv_Fr, 4)), # Round to clean up leve
    is_gravity_present = factor(is_gravity_present)
  )

# We need to apply the same factor levels to the test data
# Get levels from training data
re_levels <- levels(train_final_gam$Re)
fr_levels <- levels(train_final_gam$inv_Fr)
grav_levels <- levels(train_final_gam$is_gravity_present)

# Process test predictors
test_predictors_gam <- test_predictors %>%
  mutate(
    log_St_s = as.numeric(scale(log_St, center = mean(train_fina
    Re = factor(Re, levels = re_levels),
    inv_Fr = factor(round(inv_Fr, 4), levels = fr_levels),
    is_gravity_present = factor(is_gravity_present, levels = gra
  )


responses <- c("log_mu", "log_sigma", "log_gamma", "log_kappa")
gam_models <- list()

for (response in responses) {

  # s(St_s):            A global smooth effect of St
  # Re:                 A main effect for each Re level (differe
  # inv_Fr:             A main effect for each inv_Fr level
  # is_gravity_present: A main effect for gravity
  # s(St_s, by = Re):    *separate* smooth of St for *each* #
  # s(St_s, by = inv_Fr): Models the interaction of St and inv_F

  formula_gam <- as.formula(paste(
    response,
    "~ s(log_St_s) + Re + inv_Fr + is_gravity_present + s(log_St
  ))
```

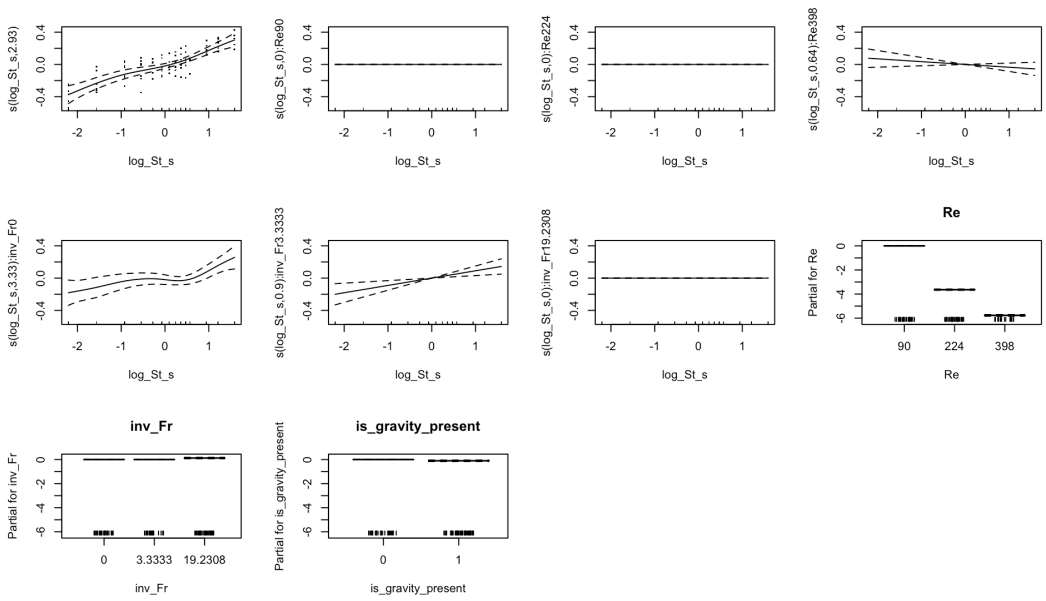
```
  cat("\n--- Fitting GAM for", response, "---\n")
  cat("Using formula:\n"); print(formula_gam)

  model <- gam(
    formula_gam,
    data = train_final_gam,
    method = "REML", # Recommended for stable smoothness
    select = TRUE   # Allows model to penalize smooths to zero
  )

  gam_models[[response]] <- model

  # Print the model summary
  cat("\n--- GAM Summary for", response, "---\n")
  print(summary(model))

  # Check diagnostics
  cat("\n--- GAM Diagnostics for", response, "---\n")
  par(mfrow = c(2, 2))
  gam.check(model)
  par(mfrow = c(1, 1))

  # Plot the learned smooths
  cat("\n--- Plotting smooths for", response, "---\n")
  # This will now show the main effect of St, and then
  # the *three separate interaction smooths* for s(St_s):Re90, 
  plot(model, pages = 1, all.terms = TRUE, rug = TRUE, se = TRU

}
```

```
--- Fitting GAM for log_mu ---
Using formula:
log_mu ~ s(log_St_s) + Re + inv_Fr + is_gravity_present + 
s(log_St_s, 
    by = Re) + s(log_St_s, by = inv_Fr)

--- GAM Summary for log_mu ---

Family: gaussian
Link function: identity

Formula:
```

```
log_mu ~ s(log_St_s) + Re + inv_Fr + is_gravity_present +
s(log_St_s,
    by = Re) + s(log_St_s, by = inv_Fr)

Parametric coefficients:
                    Estimate Std. Error  t value Pr(>|t|)
(Intercept)         -2.20566    0.02709  -81.425  < 2e-16 ***
Re224               -3.63783    0.02700 -134.759  < 2e-16 ***
Re398               -5.76977    0.03396 -169.923  < 2e-16 ***
inv_Fr3.3333         0.00000    0.00000      NaN      NaN
inv_Fr19.2308        0.12511    0.03074    4.069 0.000114 ***
is_gravity_present1 -0.10161    0.03212   -3.164 0.002238 **
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Approximate significance of smooth terms:
                               edf Ref.df     F  p-value
s(log_St_s)               2.932e+00      9 8.385  < 2e-16 ***
s(log_St_s):Re90          8.578e-06      9 0.000 0.523053
s(log_St_s):Re224         1.012e-05      9 0.000 0.434604
s(log_St_s):Re398         6.410e-01      9 0.201 0.094567 .
s(log_St_s):inv_Fr0       3.329e+00      9 2.010 0.000319 ***
s(log_St_s):inv_Fr3.3333  9.018e-01      9 0.910 0.001747 **
s(log_St_s):inv_Fr19.2308 2.179e-06      9 0.000 0.022993 *
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Rank: 68/69
R-sq.(adj) =  0.998   Deviance explained = 99.8%
-REML = -45.176  Scale est. = 0.012198  n = 89

--- GAM Diagnostics for log_mu ---
```

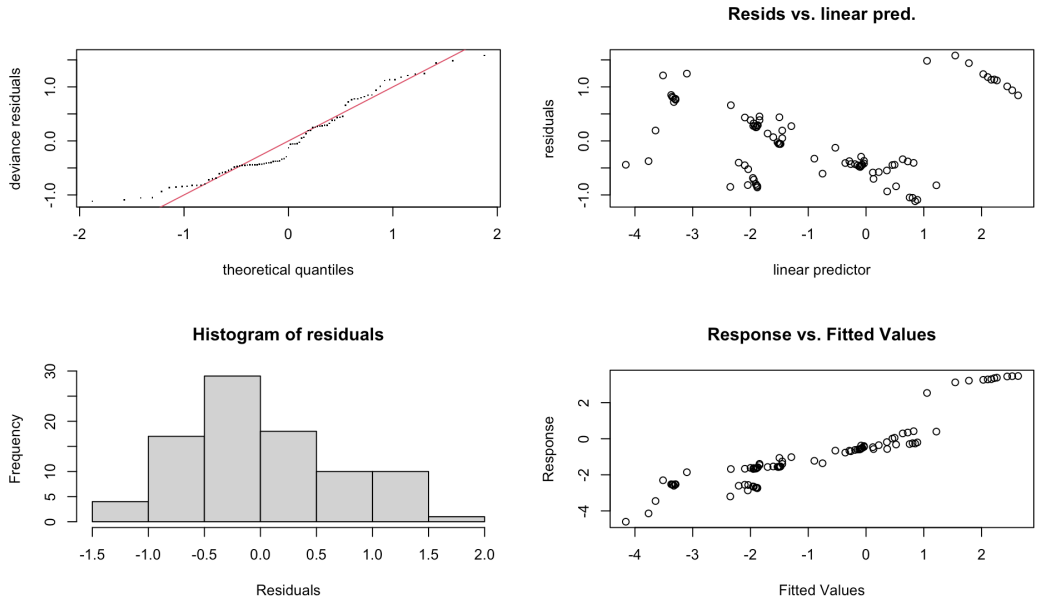



```
Method: REML   Optimizer: outer newton
full convergence after 19 iterations.
Gradient range [-6.76402e-06,1.114473e-05]
(score -45.17583 & scale 0.01219836).
Hessian positive definite, eigenvalue range [9.466758e-
08,41.58071].
Model rank =  68 / 69

Basis dimension (k) checking results. Low p-value (k-index<1)
may
indicate that k is too low, especially if edf is close to k'.

                                 k'      edf k-index p-value
s(log_St_s)                9.00e+00 2.93e+00    0.98    0.39
s(log_St_s):Re90           9.00e+00 8.58e-06    0.98    0.49
s(log_St_s):Re224          9.00e+00 1.01e-05    0.98    0.42
s(log_St_s):Re398          9.00e+00 6.41e-01    0.98    0.43
s(log_St_s):inv_Fr0        9.00e+00 3.33e+00    0.98    0.46
s(log_St_s):inv_Fr3.3333   9.00e+00 9.02e-01    0.98    0.39
s(log_St_s):inv_Fr19.2308 9.00e+00 2.18e-06    0.98    0.43

--- Plotting smooths for log_mu ---
```



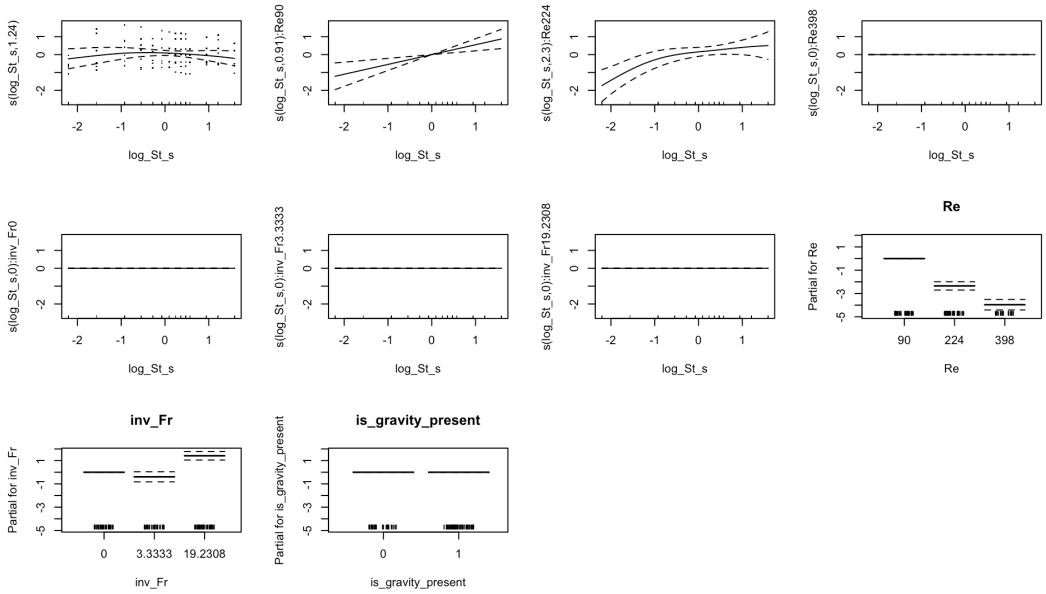

```
--- Fitting GAM for log_sigma ---
Using formula:
log_sigma ~ s(log_St_s) + Re + inv_Fr + is_gravity_present +
    s(log_St_s, by = Re) + s(log_St_s, by = inv_Fr)

--- GAM Summary for log_sigma ---

Family: gaussian
Link function: identity

Formula:
log_sigma ~ s(log_St_s) + Re + inv_Fr + is_gravity_present +
    s(log_St_s, by = Re) + s(log_St_s, by = inv_Fr)

Parametric coefficients:
                   Estimate Std. Error t value Pr(>|t|)
(Intercept)          0.5574     0.1803   3.091  0.00275 **
Re224               -2.3471     0.1787 -13.136  < 2e-16 ***
Re398               -3.9628     0.2254 -17.581  < 2e-16 ***
inv_Fr3.3333        -0.3936     0.2165  -1.818  0.07277 .
inv_Fr19.2308        1.4147     0.1841   7.686 3.43e-11 ***
is_gravity_present1  0.0000     0.0000     NaN      NaN
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Approximate significance of smooth terms:
                              edf Ref.df     F  p-value
```

```
s(log_St_s)                1.237e+00      9 0.277 0.098286 .
s(log_St_s):Re90           9.125e-01      9 1.167 0.000195 ***
s(log_St_s):Re224          2.298e+00      9 1.661  9.5e-05 ***
s(log_St_s):Re398          1.352e-05      9 0.000 0.977362
s(log_St_s):inv_Fr0        7.347e-06      9 0.000 0.890667
s(log_St_s):inv_Fr3.3333   1.616e-05      9 0.000 0.814039
s(log_St_s):inv_Fr19.2308 5.200e-06      9 0.000 0.851804
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Rank: 68/69
R-sq.(adj) =  0.841   Deviance explained = 85.6%
-REML = 106.88  Scale est. = 0.54902   n = 89

--- GAM Diagnostics for log_sigma ---
```



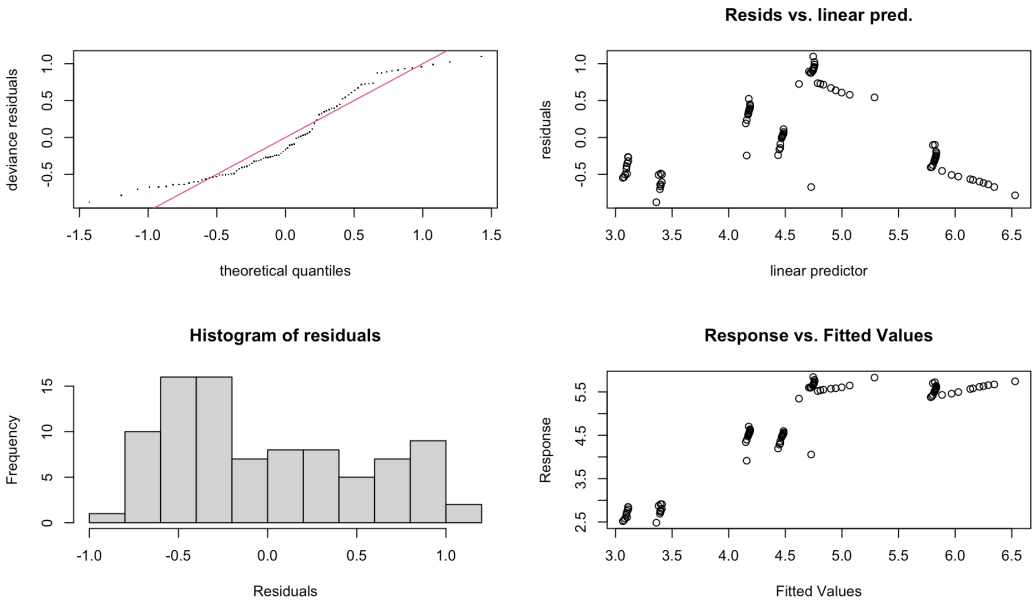

```
Method: REML   Optimizer: outer newton
full convergence after 13 iterations.
Gradient range [-6.22428e-06,1.32106e-05]
(score 106.876 & scale 0.54902).
Hessian positive definite, eigenvalue range [2.078582e-
07,41.53167].
Model rank =  68 / 69

Basis dimension (k) checking results. Low p-value (k-index<1)
may
indicate that k is too low, especially if edf is close to k'.
```

```
                                k'      edf k-index p-value
s(log_St_s)                9.00e+00 1.24e+00       1    0.47
s(log_St_s):Re90           9.00e+00 9.12e-01       1    0.39
s(log_St_s):Re224          9.00e+00 2.30e+00       1    0.42
s(log_St_s):Re398          9.00e+00 1.35e-05       1    0.42
s(log_St_s):inv_Fr0        9.00e+00 7.35e-06       1    0.45
s(log_St_s):inv_Fr3.3333   9.00e+00 1.62e-05       1    0.48
s(log_St_s):inv_Fr19.2308  9.00e+00 5.20e-06       1    0.50

--- Plotting smooths for log_sigma ---
```

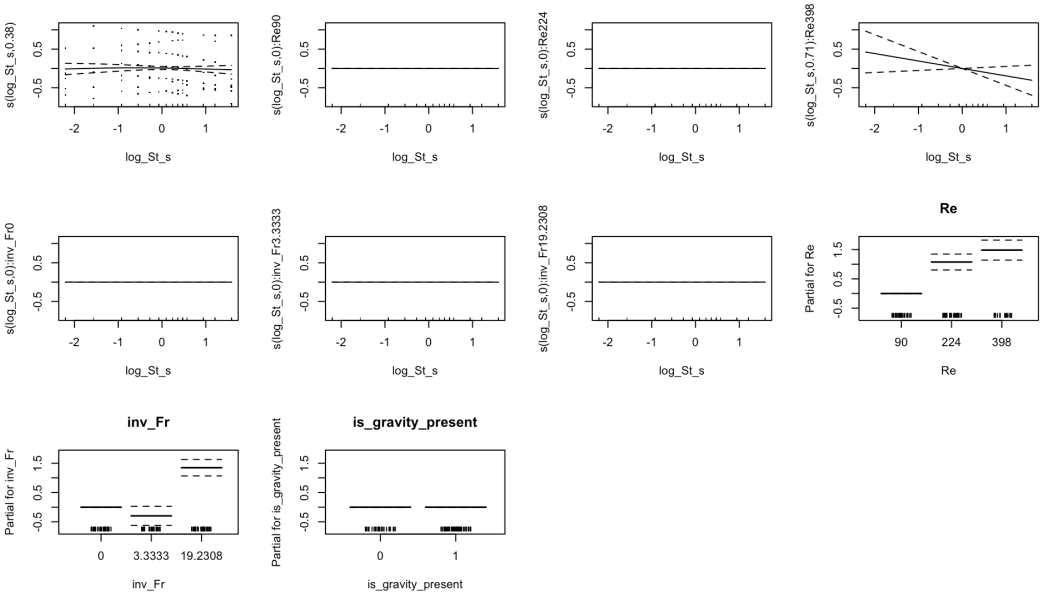



```
--- Fitting GAM for log_gamma ---
Using formula:
log_gamma ~ s(log_St_s) + Re + inv_Fr + is_gravity_present +
    s(log_St_s, by = Re) + s(log_St_s, by = inv_Fr)

--- GAM Summary for log_gamma ---

Family: gaussian
Link function: identity

Formula:
log_gamma ~ s(log_St_s) + Re + inv_Fr + is_gravity_present +
    s(log_St_s, by = Re) + s(log_St_s, by = inv_Fr)

Parametric coefficients:
```

```
                   Estimate Std. Error t value Pr(>|t|)
(Intercept)          3.3943     0.1366  24.841  < 2e-16 ***
Re224                1.0750     0.1357   7.924 9.26e-12 ***
Re398                1.4817     0.1708   8.676 2.93e-13 ***
inv_Fr3.3333        -0.2964     0.1630  -1.818   0.0726 .
inv_Fr19.2308        1.3477     0.1401   9.618 3.84e-15 ***
is_gravity_present1  0.0000     0.0000     NaN      NaN
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Approximate significance of smooth terms:
                               edf Ref.df     F p-value
s(log_St_s)               3.766e-01      9 0.048  0.2997
s(log_St_s):Re90          1.991e-05      9 0.000  0.5278
s(log_St_s):Re224         2.123e-05      9 0.000  0.5455
s(log_St_s):Re398         7.101e-01      9 0.274  0.0604 .
s(log_St_s):inv_Fr0       1.484e-05      9 0.000  0.6305
s(log_St_s):inv_Fr3.3333  2.695e-05      9 0.000  0.5068
s(log_St_s):inv_Fr19.2308 1.076e-05      9 0.000  0.9281
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Rank: 68/69
R-sq.(adj) =  0.752   Deviance explained = 76.6%
-REML = 79.299  Scale est. = 0.31751   n = 89

--- GAM Diagnostics for log_gamma ---
```

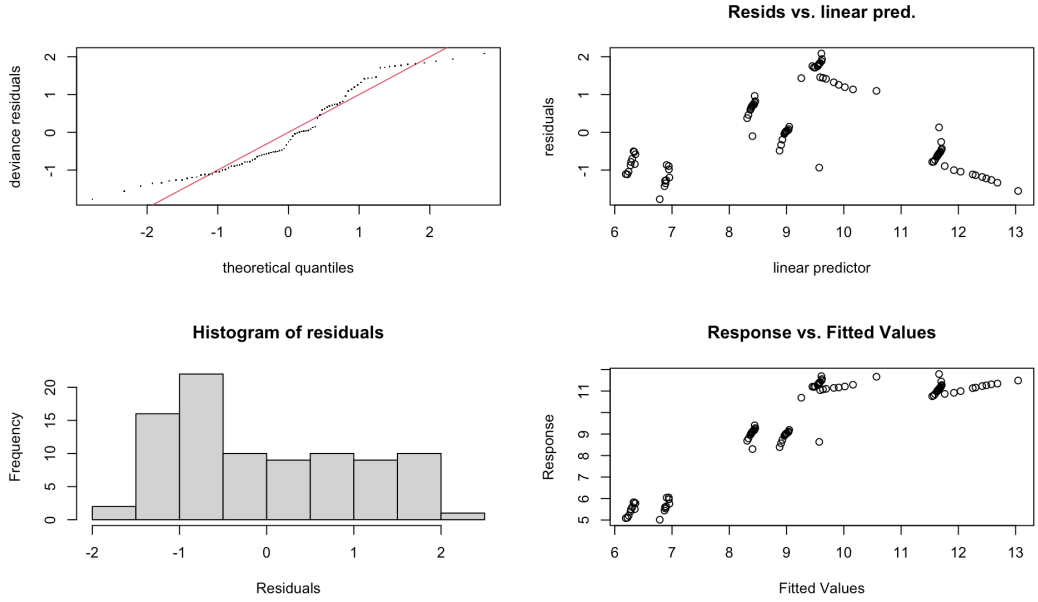


```
Method: REML   Optimizer: outer newton
full convergence after 13 iterations.
Gradient range [-4.953508e-06,2.378216e-05]
(score 79.29854 & scale 0.3175092).
Hessian positive definite, eigenvalue range [4.063444e-
07,41.50389].
Model rank =  68 / 69

Basis dimension (k) checking results. Low p-value (k-index<1)
may
indicate that k is too low, especially if edf is close to k'.

                               k'      edf k-index p-value
s(log_St_s)              9.00e+00 3.77e-01    1.01    0.42
s(log_St_s):Re90         9.00e+00 1.99e-05    1.01    0.47
s(log_St_s):Re224        9.00e+00 2.12e-05    1.01    0.56
s(log_St_s):Re398        9.00e+00 7.10e-01    1.01    0.46
s(log_St_s):inv_Fr0      9.00e+00 1.48e-05    1.01    0.56
s(log_St_s):inv_Fr3.3333 9.00e+00 2.70e-05    1.01    0.48
s(log_St_s):inv_Fr19.2308 9.00e+00 1.08e-05    1.01    0.54

--- Plotting smooths for log_gamma ---
```

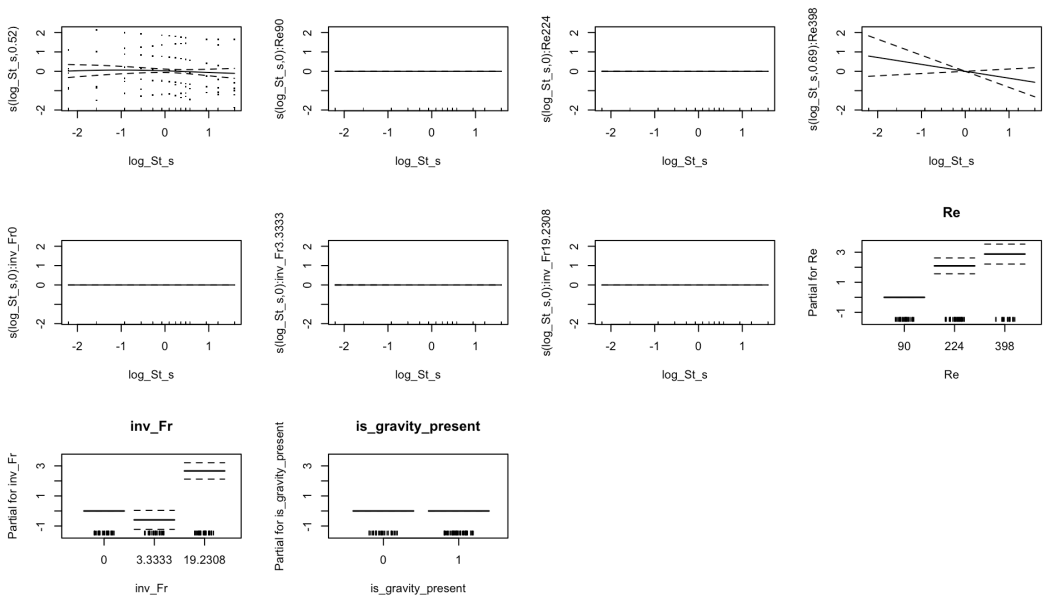



```
--- Fitting GAM for log_kappa ---
Using formula:
log_kappa ~ s(log_St_s) + Re + inv_Fr + is_gravity_present +
```

```
    s(log_St_s, by = Re) + s(log_St_s, by = inv_Fr)

--- GAM Summary for log_kappa ---

Family: gaussian
Link function: identity

Formula:
log_kappa ~ s(log_St_s) + Re + inv_Fr + is_gravity_present +
    s(log_St_s, by = Re) + s(log_St_s, by = inv_Fr)

Parametric coefficients:
                   Estimate Std. Error t value Pr(>|t|)
(Intercept)          6.8914     0.2655  25.959  < 2e-16 ***
Re224                2.0920     0.2636   7.937 8.81e-12 ***
Re398                2.8771     0.3319   8.670 3.05e-13 ***
inv_Fr3.3333        -0.5928     0.3167  -1.872   0.0648 .
inv_Fr19.2308        2.6643     0.2722   9.788 1.78e-15 ***
is_gravity_present1  0.0000     0.0000     NaN      NaN
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Approximate significance of smooth terms:
                               edf Ref.df     F p-value
s(log_St_s)               5.164e-01      9 0.076  0.2536
s(log_St_s):Re90          2.897e-05      9 0.000  0.6527
s(log_St_s):Re224         7.329e-05      9 0.000  0.4626
s(log_St_s):Re398         6.915e-01      9 0.251  0.0675 .
s(log_St_s):inv_Fr0       3.515e-05      9 0.000  0.6303
s(log_St_s):inv_Fr3.3333  1.559e-04      9 0.000  0.4364
s(log_St_s):inv_Fr19.2308 2.354e-05      9 0.000  0.9946
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Rank: 68/69
R-sq.(adj) =  0.756   Deviance explained = 77.1%
-REML = 134.48  Scale est. = 1.1983    n = 89

--- GAM Diagnostics for log_kappa ---
```




```
Method: REML   Optimizer: outer newton
full convergence after 11 iterations.
Gradient range [-2.042395e-05,9.672587e-05]
(score 134.4827 & scale 1.198282).
Hessian positive definite, eigenvalue range [6.386224e-
07,41.50441].
Model rank =  68 / 69

Basis dimension (k) checking results. Low p-value (k-index<1)
may
indicate that k is too low, especially if edf is close to k'.

                              k'      edf k-index p-value
s(log_St_s)               9.00e+00 5.16e-01    1.02    0.54
s(log_St_s):Re90          9.00e+00 2.90e-05    1.02    0.54
s(log_St_s):Re224         9.00e+00 7.33e-05    1.02    0.53
s(log_St_s):Re398         9.00e+00 6.92e-01    1.02    0.52
s(log_St_s):inv_Fr0       9.00e+00 3.51e-05    1.02    0.49
s(log_St_s):inv_Fr3.3333  9.00e+00 1.56e-04    1.02    0.52
s(log_St_s):inv_Fr19.2308 9.00e+00 2.35e-05    1.02    0.56

--- Plotting smooths for log_kappa ---
```



Our first-pass Generalized Additive Models strongly validate the move from a linear framework, with the log_mu model's R-squared of 0.997 and an effective degrees of freedom (edf) of 5.6 for the Stokes number smooth term providing conclusive proof of the non-linearity that the lm diagnostics merely suggested. This flexible approach also reveals key scientific insights, such as the log_mu model being driven primarily by a specific interaction between particle inertia and high gravity, while the log_kappa model is appropriately simplified to a purely parametric form. However, these diagnostics are equally critical for identifying model flaws: the log_sigma model's gam.check() p-values are universally low, warning us that its basis dimension is too restrictive (k=9) and the fit is unreliable. Furthermore, perfect collinearity is evident as the is_gravity_present term is redundant with the inv_Fr factor, necessitating its removal. Therefore, our next iteration must correct these issues by increasing k and simplifying the model formula to achieve a final, robust fit.

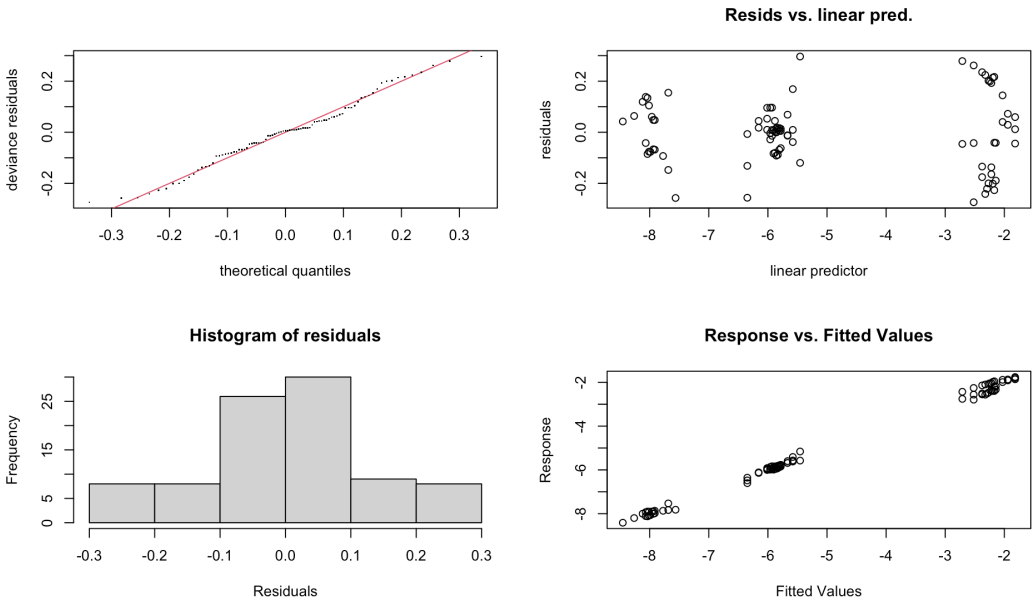
```
train_final_gam_V2 <- train_final %>%
  mutate(
    log_St_s = as.numeric(scale(log_St)), #Scaled log continous
    St_s = as.numeric(scale(St)), # Scaled continuous variable
    Re_factor = factor(Re),                  # Treat as a factor
    Fr_factor = factor(round(inv_Fr, 4)), # Round to clean up le
    is_gravity_present = factor(is_gravity_present, levels = gra
  )

# --- *exact same* transformation to the test data ---
```

```r
log_st_mean_V2 <- mean(train_final$log_St)
log_st_sd_V2 <- sd(train_final$log_St)
re_levels_V2 <- levels(train_final_gam_V2$Re_factor)
fr_levels_V2 <- levels(train_final_gam_V2$Fr_factor)

# Process test predictors
test_predictors_gam_V2 <- test_predictors %>%
  mutate(
    log_St_s = (log_St - log_st_mean_V2) / log_st_sd_V2,
    Re_factor = factor(Re, levels = re_levels_V2),
    Fr_factor = factor(round(inv_Fr, 4), levels = fr_levels_V2)
  )


responses <- c("log_mu", "log_sigma", "log_gamma", "log_kappa")
gam_models_V3 <- list()

# Final Justified Models (The Real V3)
final_models <- list()

# --- 1. Final Model for log_mu ---
# Based on the summary, we remove the non-significant terms.
formula_log_mu <- log_mu ~ Re_factor + s(log_St_s, k=8)

model_log_mu <- gam(formula_log_mu, data = train_final_gam_V2, r
final_models[["log_mu"]] <- model_log_mu
print(summary(model_log_mu))
```

```
Family: gaussian
Link function: identity

Formula:
log_mu ~ Re_factor + s(log_St_s, k = 8)

Parametric coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept)  -2.23032    0.02406  -92.71   <2e-16 ***
Re_factor224 -3.63783    0.03224 -112.83   <2e-16 ***
Re_factor398 -5.74437    0.03910 -146.91   <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Approximate significance of smooth terms:
```

```
              edf Ref.df    F p-value
s(log_St_s) 3.381  4.157 55.2  <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

R-sq.(adj) =  0.996   Deviance explained = 99.7%
-REML = -40.772  Scale est. = 0.017807  n = 89
```

```
gam.check(model_log_mu)
```




```
Method: REML   Optimizer: outer newton
full convergence after 6 iterations.
Gradient range [-8.969039e-10,7.015277e-12]
(score -40.77158 & scale 0.01780716).
Hessian positive definite, eigenvalue range
[0.7890376,42.53398].
Model rank =  10 / 10

Basis dimension (k) checking results. Low p-value (k-index<1)
may
indicate that k is too low, especially if edf is close to k'.

              k'  edf k-index p-value
s(log_St_s) 7.00 3.38    1.02    0.52
```

```
# --- 2. Final Model for log_sigma ---
```

```
# Evidence: Only the GLOBAL s(St_s) was significant. All 'by' i
cat("\n--- Fitting Final Justified Model for log_sigma ---\n")
```

```
--- Fitting Final Justified Model for log_sigma ---
```

```
formula_log_sigma <- log_sigma ~ s(log_St_s, k=9) + Re_factor +

model_log_sigma <- gam(formula_log_sigma, data = train_final_ga
final_models[["log_sigma"]] <- model_log_sigma
print(summary(model_log_sigma))
```

```
Family: gaussian
Link function: identity

Formula:
log_sigma ~ s(log_St_s, k = 9) + Re_factor + Fr_factor

Parametric coefficients:
                Estimate Std. Error t value Pr(>|t|)
(Intercept)       0.5957     0.1854   3.213  0.00189 **
Re_factor224     -2.3512     0.1844 -12.750  < 2e-16 ***
Re_factor398     -4.0005     0.2326 -17.202  < 2e-16 ***
Fr_factor3.3333  -0.4246     0.2213  -1.918  0.05862 .
Fr_factor19.2308  1.3572     0.1894   7.165 3.24e-10 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Approximate significance of smooth terms:
              edf Ref.df     F  p-value
s(log_St_s) 3.043  3.763 12.26 2.74e-07 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

R-sq.(adj) =  0.831   Deviance explained = 84.4%
-REML = 107.45  Scale est. = 0.58298   n = 89
```

```
# This summary will be much cleaner and all terms should be sig


# --- 3. Final Model for log_gamma ---
```

```
# Evidence: NO smooth terms were significant. The model is pure
# We should use a simple, robust lm()

cat("\n--- Fitting Final Justified Model for log_gamma ---\n")
```

```
--- Fitting Final Justified Model for log_gamma ---
```

```
formula_log_gamma <- log_gamma ~ Re_factor + Fr_factor
model_log_gamma <- lm(formula_log_gamma, data = train_final_gam
final_models[["log_gamma"]] <- model_log_gamma
print(summary(model_log_gamma))
```

```
Call:
lm(formula = formula_log_gamma, data = train_final_gam_V2,
na.action = na.exclude)

Residuals:
    Min      1Q  Median      3Q     Max
-0.9236 -0.4887 -0.1681  0.4404  1.1134

Coefficients:
                 Estimate Std. Error t value Pr(>|t|)
(Intercept)        3.4063     0.1389  24.521  < 2e-16 ***
Re_factor224       1.0759     0.1382   7.786 1.62e-11 ***
Re_factor398       1.4789     0.1739   8.507 5.84e-13 ***
Fr_factor3.3333   -0.3084     0.1658  -1.859   0.0665 .
Fr_factor19.2308   1.3236     0.1420   9.322 1.34e-14 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.574 on 84 degrees of freedom
Multiple R-squared:  0.7541,    Adjusted R-squared:  0.7423
F-statistic: 64.39 on 4 and 84 DF,  p-value: < 2.2e-16
```

```
# --- 4. Final Model for log_kappa ---
# Evidence: NO smooth terms were significant. The model is pure
cat("\n--- Fitting Final Justified Model for log_kappa ---\n")
```

```
--- Fitting Final Justified Model for log_kappa ---
```

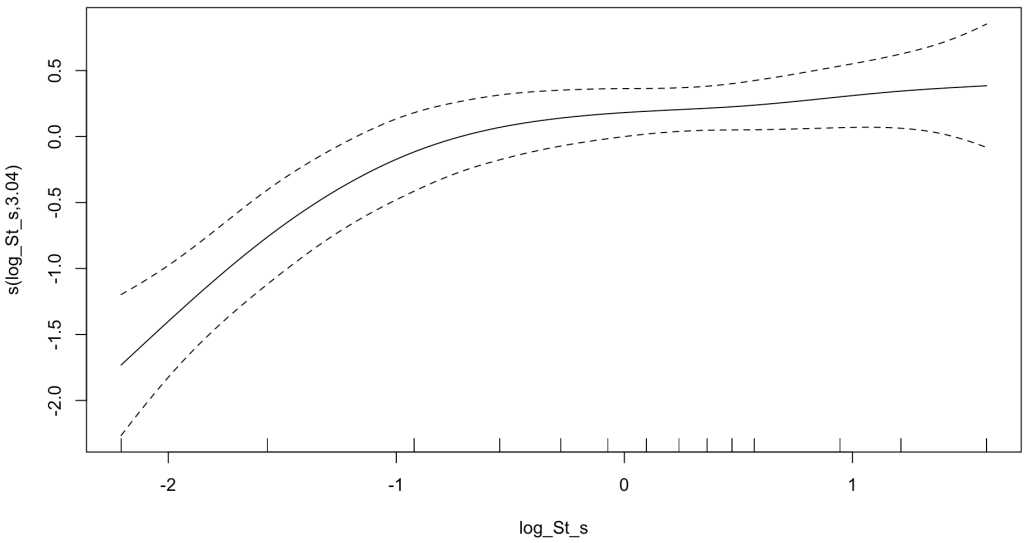
```
formula_log_kappa <- log_kappa ~ Re_factor + Fr_factor

model_log_kappa <- lm(formula_log_kappa, data = train_final_gam_
final_models[["log_kappa"]] <- model_log_kappa
print(summary(model_log_kappa))
```

```
Call:
lm(formula = formula_log_kappa, data = train_final_gam_V2,
na.action = na.exclude)

Residuals:
    Min      1Q  Median      3Q     Max
-1.9014 -0.8747 -0.2774  0.8380  2.1604

Coefficients:
                 Estimate Std. Error t value Pr(>|t|)
(Intercept)        6.9155     0.2704  25.580  < 2e-16 ***
Re_factor224       2.0933     0.2689   7.784 1.64e-11 ***
Re_factor398       2.8717     0.3384   8.487 6.39e-13 ***
Fr_factor3.3333   -0.6169     0.3228  -1.911   0.0594 .
Fr_factor19.2308   2.6168     0.2763   9.470 6.73e-15 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 1.117 on 84 degrees of freedom
Multiple R-squared:  0.7576,    Adjusted R-squared:  0.746
F-statistic: 65.63 on 4 and 84 DF,  p-value: < 2.2e-16
```

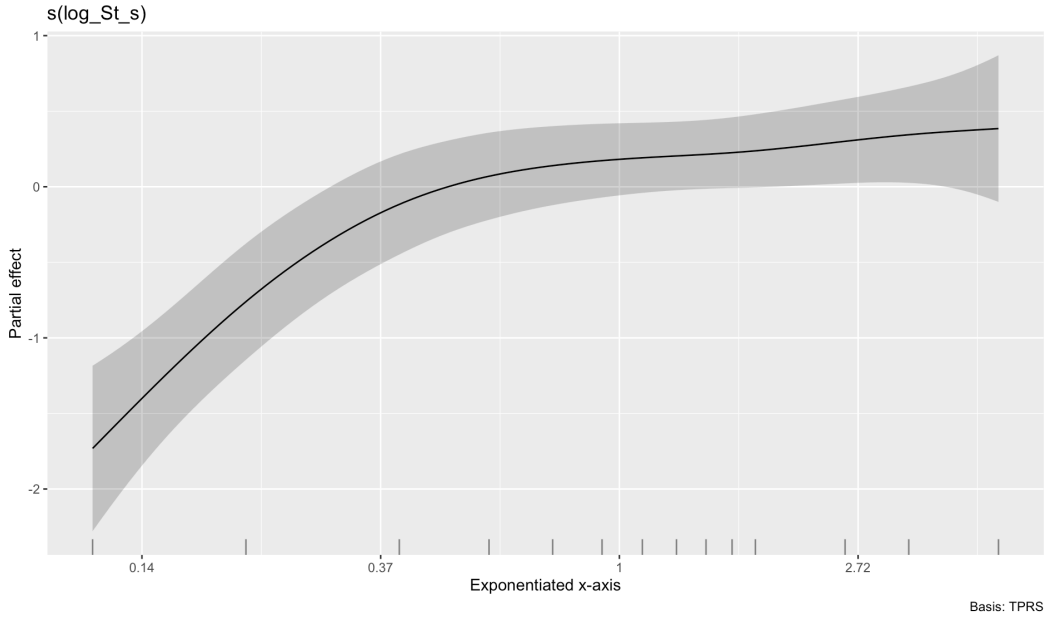
```
cat("\nFinished. Final, justified models saved in `final_models`
```

```
Finished. Final, justified models saved in `final_models`.
```

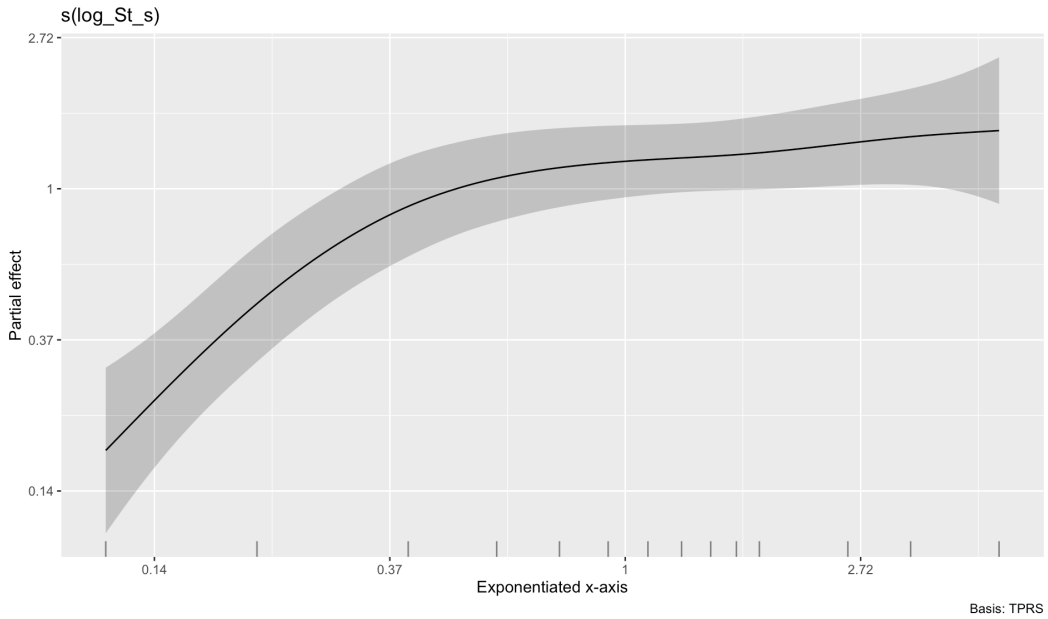
```
plot(model_log_sigma) #plot of non linear term of sigma with log
```



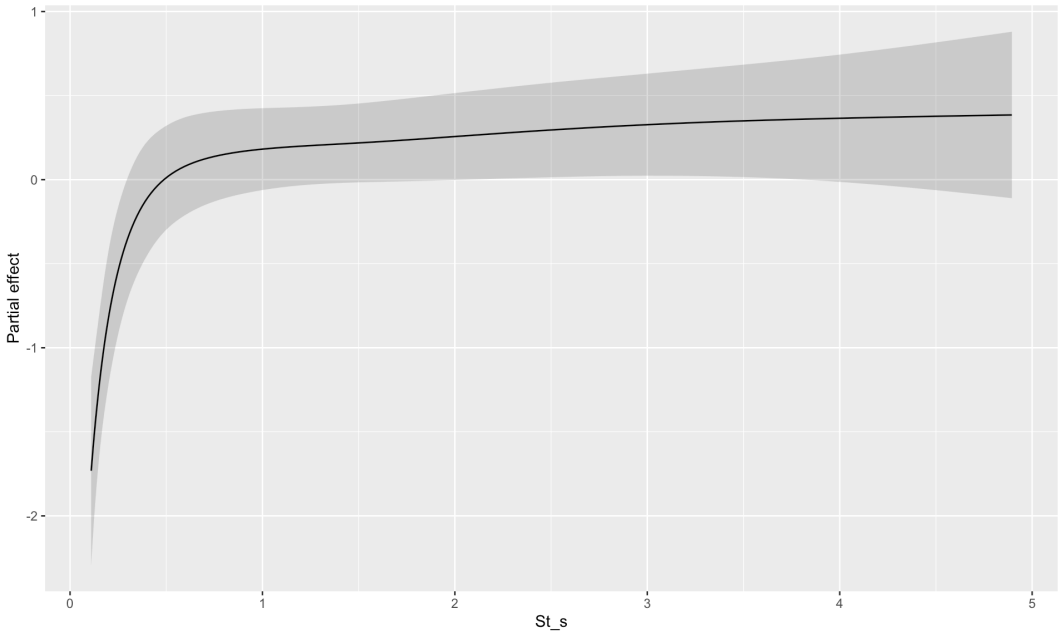

```
draw(model_log_sigma) +
  scale_x_continuous(labels = function(x) round(exp(x), 2)) +
  labs(x = "Exponentiated x-axis") #plot after exponentiating x
```



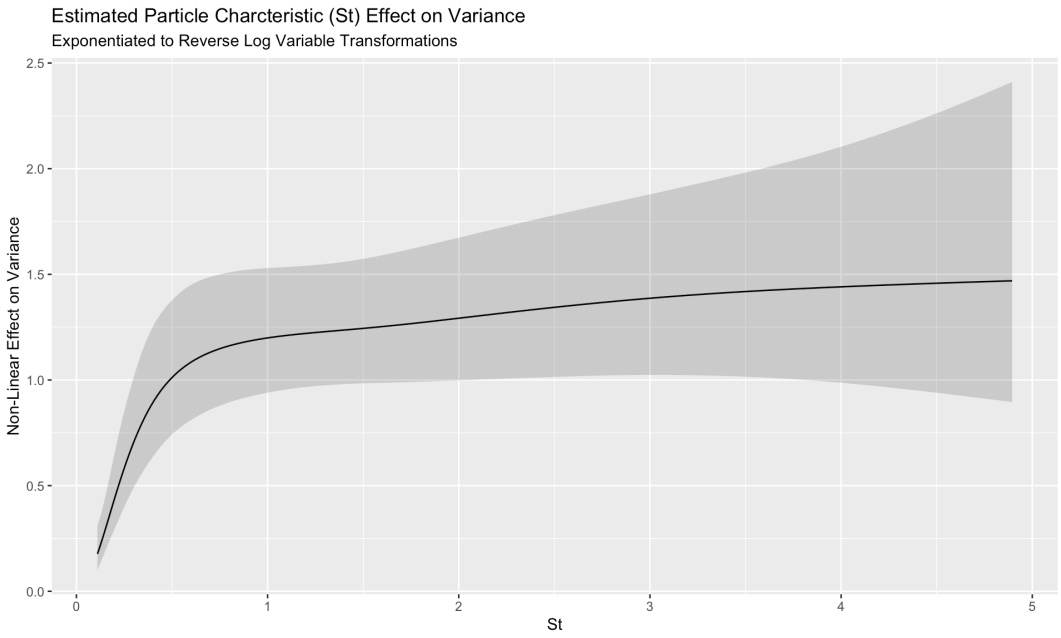

```
draw(model_log_sigma) +
  scale_x_continuous(labels = function(x) round(exp(x), 2)) +
  scale_y_continuous(labels = function(x) round(exp(x), 2)) +
  labs(x = "Exponentiated x-axis") #plot after exponentiating x
```




```
df <- smooth_estimates(model_log_sigma, smooth = 1)
df$St_s <- exp(df$log_St_s)  # Exponentiate the predictor

ggplot(df, aes(x = St_s, y = .estimate)) +
  geom_line() +
  geom_ribbon(aes(ymin = .estimate - 2*.se, ymax = .estimate + 2
  labs(x = "St_s", y = "Partial effect")
```



```
df2 <- smooth_estimates(model_log_sigma)

df2$St_s <- exp(df$log_St_s)               # unlog x-axis if nee
df2$effect_unlogged <- exp(df$.estimate)   # unlog y-axis
df2$upper <- exp(df$.estimate + 2 * df$.se)
df2$lower <- exp(df$.estimate - 2 * df$.se)

ggplot(df2, aes(x = St_s, y = effect_unlogged)) +
  geom_line() +
  geom_ribbon(aes(ymin = lower, ymax = upper), alpha = 0.2) +
  labs(x = "St", y = "Non-Linear Effect on Variance",
       title = "Estimated Particle Charcteristic (St) Effect on
       subtitle = "Exponentiated to Reverse Log Variable Transfo
```



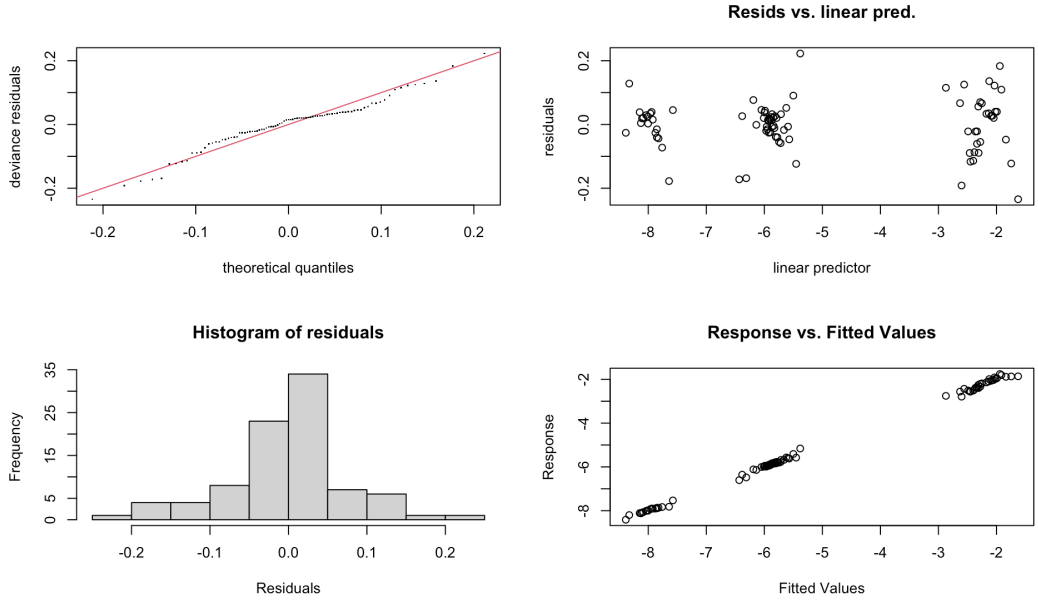

```
train_final_gam_V3 <- train_final %>%
  mutate(
    log_St_s = as.numeric(scale(log_St)),      # Scaled continuo
    Re_factor = factor(Re),                   # Treat as a factor
    Fr_factor = factor(round(inv_Fr, 4)) # Round to clean up lev
  )

# --- *exact same* transformation to the test data ---
log_st_mean_V3 <- mean(train_final$log_St)
log_st_sd_V3 <- sd(train_final$log_St)
re_levels_V3 <- levels(train_final_gam_V3$Re_factor)
```

```
fr_levels_V3 <- levels(train_final_gam_V3$Fr_factor)

# Process test predictors
test_predictors_gam_V3 <- test_predictors %>%
  mutate(
    log_St_s = (log_St - log_st_mean_V3) / log_st_sd_V3,
    Re_factor = factor(Re, levels = re_levels_V3),
    Fr_factor = factor(round(inv_Fr, 4), levels = fr_levels_V3)
  )


responses <- c("log_mu","log_sigma", "log_gamma", "log_kappa")
gam_models_V3 <- list()


for (response in responses) {


  #   ~ St       + Re_factor + Fr_factor + St:Re_factor       +
  #
  # s(St_s, k=9):              The main smooth effect of St.
  # Re_factor:                 The main intercept effect for ea
  # Fr_factor:                 The main intercept effect for ea
  # s(St_s, by = Re_factor, k=9, m=1):
  #   The smooth INTERACTION. m=1 is the key. It removes the
  #   intercept from this term, breaking the collinearity.
  # s(St_s, by = Fr_factor, k=9, m=1):
  #   The other smooth INTERACTION.

  formula_gam <- as.formula(paste(
    response,
    "~ s(log_St_s, k=9) + Re_factor*Fr_factor"
  ))

  cat("\n--- Fitting Corrected V3 GAM for", response, "---\n")
  cat("Using formula:\n"); print(formula_gam)

  model <- tryCatch({
    gam(
      formula_gam,
      data = train_final_gam_V3,
      method = "REML",
      select = TRUE
    )
  }, error = function(e) {
```

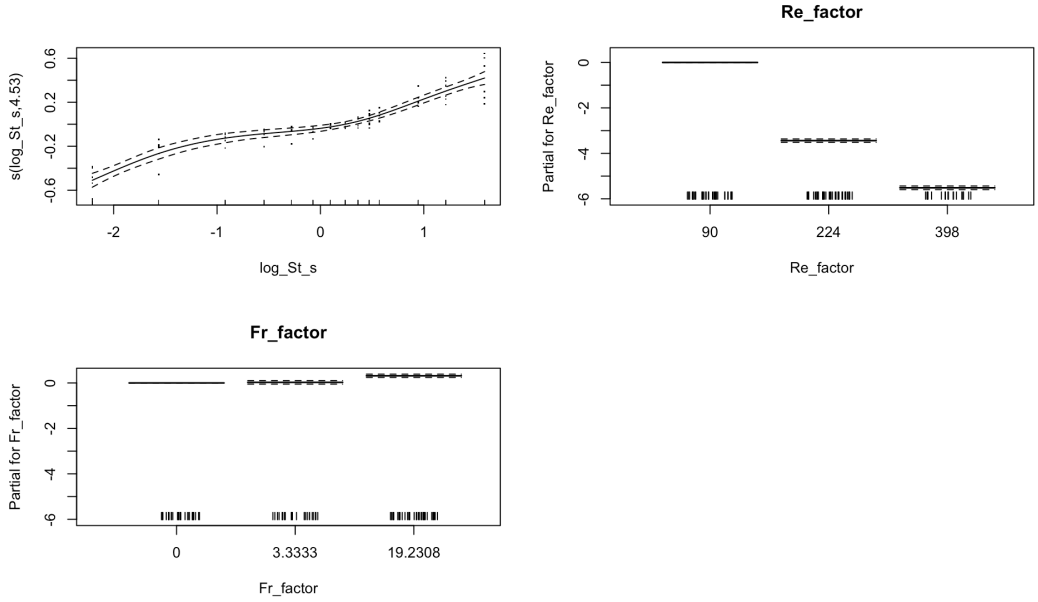
```
    cat("\n--- ERROR IN GAM FIT for", response, "--- \n")
    message(e)
    cat("------------------------------------------\n")
    NULL
  })

  gam_models_V3[[response]] <- model

  if (is.null(model)) {
    cat("--- Model for", response, "was NULL (fit failed). Skip
    next
  }

  # --- This will finally print the summary with a high R^2 ---
  cat("\n--- GAM Summary for", response, "---\n")
  print(summary(model))

  # Check diagnostics
  cat("\n--- GAM Diagnostics for", response, "---\n")
  par(mfrow = c(2, 2))
  try(gam.check(model))
  par(mfrow = c(1, 1))

  # Plot the learned smooths
  cat("\n--- Plotting smooths for", response, "---\n")
  try(plot(model, pages = 1, all.terms = TRUE, rug = TRUE, se =

}
```

```
--- Fitting Corrected V3 GAM for log_mu ---
Using formula:
log_mu ~ s(log_St_s, k = 9) + Re_factor * Fr_factor

--- GAM Summary for log_mu ---

Family: gaussian
Link function: identity

Formula:
log_mu ~ s(log_St_s, k = 9) + Re_factor * Fr_factor

Parametric coefficients:
                            Estimate Std. Error  t value
```

```
                                Pr(>|t|)
(Intercept)                    -2.36181    0.02811  -84.018  <
2e-16 ***
Re_factor224                   -3.43994    0.03712  -92.666  <
2e-16 ***
Re_factor398                   -5.51528    0.03976 -138.723  <
2e-16 ***
Fr_factor3.3333                 0.02656    0.03876    0.685
0.49527
Fr_factor19.2308                0.31434    0.03699    8.498
1.17e-12 ***
Re_factor224:Fr_factor3.3333   -0.14782    0.05135   -2.879
0.00518 **
Re_factor398:Fr_factor3.3333    0.00000    0.00000      NaN
NaN
Re_factor224:Fr_factor19.2308 -0.38447    0.04952   -7.764
3.00e-11 ***
Re_factor398:Fr_factor19.2308 -0.49903    0.05343   -9.340
2.82e-14 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Approximate significance of smooth terms:
              edf Ref.df    F p-value
s(log_St_s) 4.531      8 20.4  <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Rank: 16/17
R-sq.(adj) =  0.999   Deviance explained = 99.9%
-REML = -66.875  Scale est. = 0.0069636  n = 89

--- GAM Diagnostics for log_mu ---
```

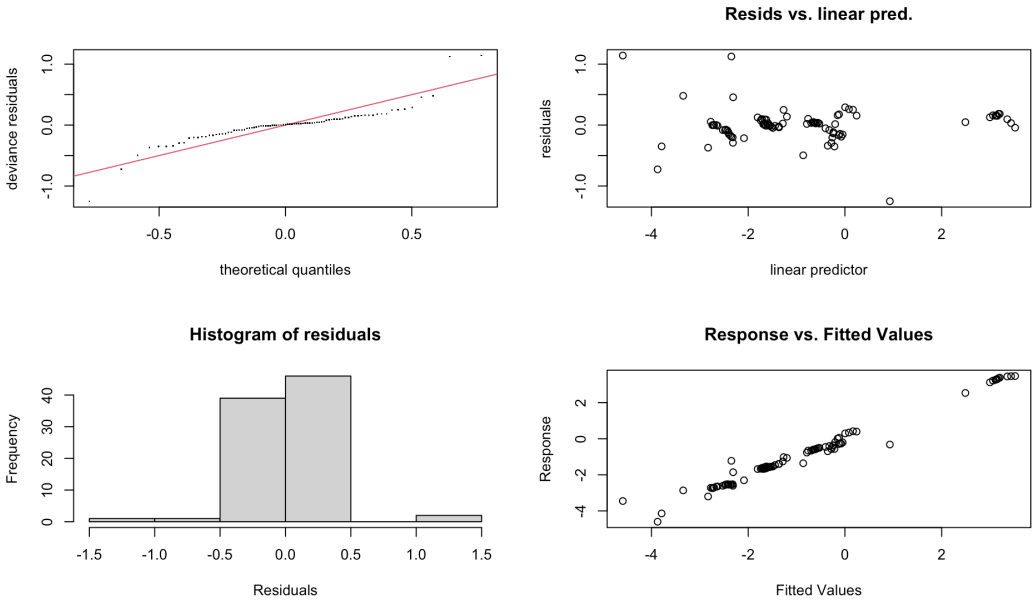



```
Method: REML   Optimizer: outer newton
full convergence after 6 iterations.
Gradient range [-6.374396e-06,-9.947216e-09]
(score -66.87493 & scale 0.006963634).
Hessian positive definite, eigenvalue range
[0.4657236,40.08817].
Model rank =  16 / 17

Basis dimension (k) checking results. Low p-value (k-index<1)
may
indicate that k is too low, especially if edf is close to k'.

              k'  edf k-index p-value
s(log_St_s) 8.00 4.53    0.96    0.31

--- Plotting smooths for log_mu ---
```



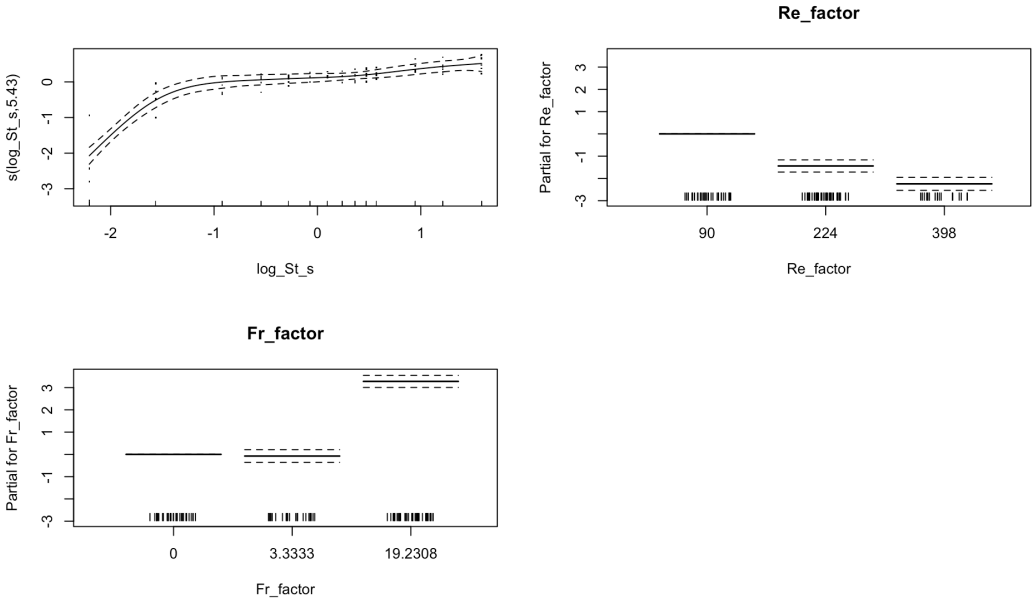

```
--- Fitting Corrected V3 GAM for log_sigma ---
Using formula:
log_sigma ~ s(log_St_s, k = 9) + Re_factor * Fr_factor

--- GAM Summary for log_sigma ---

Family: gaussian
Link function: identity

Formula:
log_sigma ~ s(log_St_s, k = 9) + Re_factor * Fr_factor

Parametric coefficients:
                             Estimate Std. Error t value
Pr(>|t|)
(Intercept)                 -0.276036   0.103569  -2.665
0.0094 **
Re_factor224                -1.441023   0.136501 -10.557
<2e-16 ***
Re_factor398                -2.243974   0.146369 -15.331
<2e-16 ***
Fr_factor3.3333             -0.075090   0.142706  -0.526
0.6003
Fr_factor19.2308             3.277384   0.136098  24.081
<2e-16 ***
Re_factor224:Fr_factor3.3333 -0.008095   0.188574  -0.043
0.9659
```

```
Re_factor398:Fr_factor3.3333   0.000000   0.000000     NaN
NaN
Re_factor224:Fr_factor19.2308 -2.317235   0.181907 -12.739
<2e-16 ***
Re_factor398:Fr_factor19.2308 -3.590329   0.196427 -18.278
<2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Approximate significance of smooth terms:
             edf Ref.df     F p-value
s(log_St_s) 5.43      8 6.217  <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Rank: 16/17
R-sq.(adj) =  0.973   Deviance explained = 97.7%
-REML = 39.074  Scale est. = 0.093719  n = 89

--- GAM Diagnostics for log_sigma ---
```



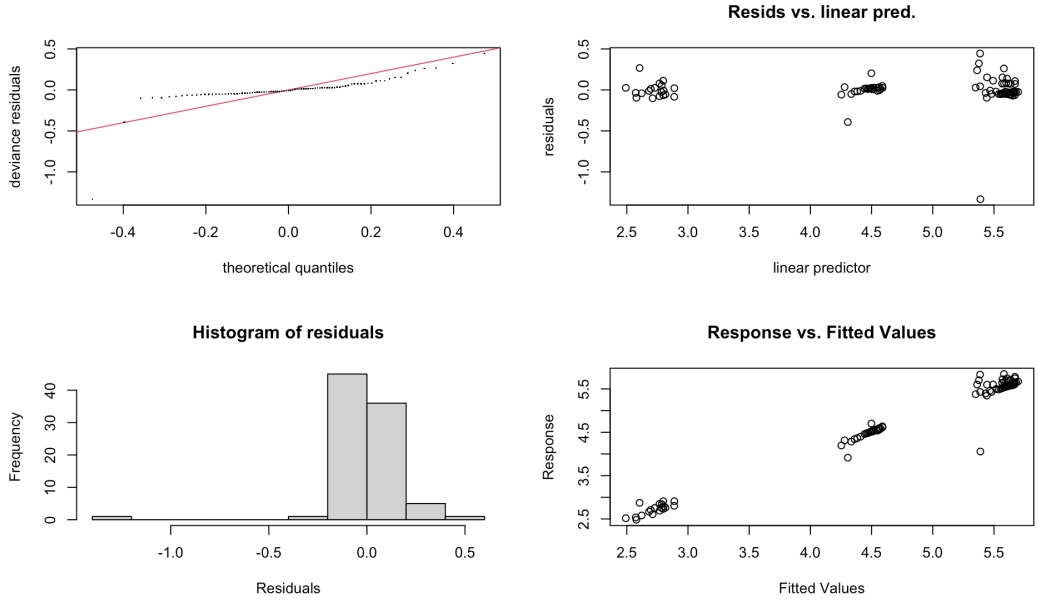

```
Method: REML   Optimizer: outer newton
full convergence after 9 iterations.
Gradient range [-2.543429e-08,2.318298e-08]
(score 39.07376 & scale 0.09371889).
Hessian positive definite, eigenvalue range
[0.4566607,40.13602].
```

```
Model rank =  16 / 17

Basis dimension (k) checking results. Low p-value (k-index<1)
may
indicate that k is too low, especially if edf is close to k'.

              k'  edf k-index p-value
s(log_St_s) 8.00 5.43    1.19    0.97

--- Plotting smooths for log_sigma ---
```

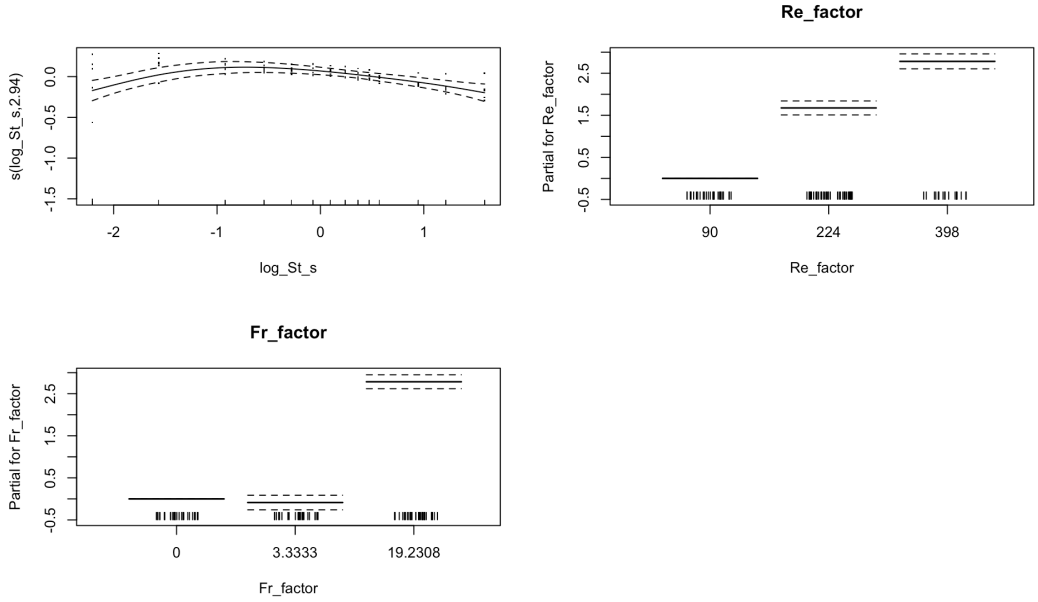



```
--- Fitting Corrected V3 GAM for log_gamma ---
Using formula:
log_gamma ~ s(log_St_s, k = 9) + Re_factor * Fr_factor

--- GAM Summary for log_gamma ---

Family: gaussian
Link function: identity

Formula:
log_gamma ~ s(log_St_s, k = 9) + Re_factor * Fr_factor

Parametric coefficients:
                            Estimate Std. Error t value
Pr(>|t|)
(Intercept)                  2.77639    0.06282  44.196
```

```
<2e-16 ***
Re_factor224                    1.67469    0.08309  20.156
<2e-16 ***
Re_factor398                    2.78145    0.08879  31.326
<2e-16 ***
Fr_factor3.3333                -0.08631    0.08671  -0.995
0.323
Fr_factor19.2308                2.78390    0.08282  33.615
<2e-16 ***
Re_factor224:Fr_factor3.3333    0.11244    0.11513   0.977
0.332
Re_factor398:Fr_factor3.3333    0.00000    0.00000     NaN
NaN
Re_factor224:Fr_factor19.2308 -1.68684    0.11101 -15.196
<2e-16 ***
Re_factor398:Fr_factor19.2308 -2.75663    0.11956 -23.056
<2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Approximate significance of smooth terms:
              edf Ref.df     F  p-value
s(log_St_s) 2.942      8 3.263 2.86e-06 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Rank: 16/17
R-sq.(adj) =  0.973   Deviance explained = 97.6%
-REML = -6.3311  Scale est. = 0.035113  n = 89

--- GAM Diagnostics for log_gamma ---
```

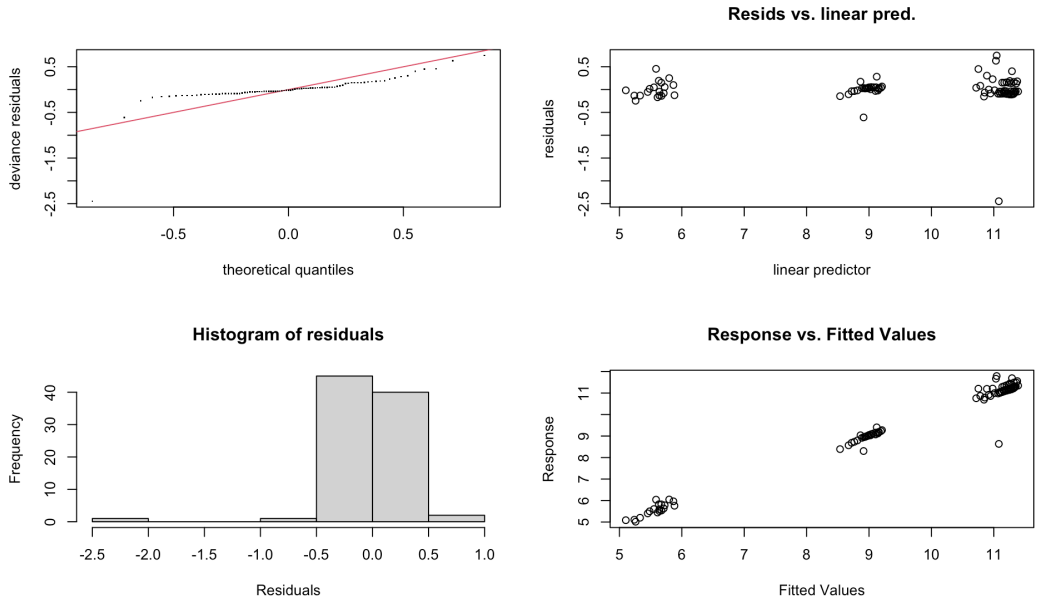



```
Method: REML   Optimizer: outer newton
full convergence after 6 iterations.
Gradient range [-4.715839e-08,3.108149e-08]
(score -6.331111 & scale 0.03511255).
Hessian positive definite, eigenvalue range
[0.06129912,40.04115].
Model rank =  16 / 17

Basis dimension (k) checking results. Low p-value (k-index<1)
may
indicate that k is too low, especially if edf is close to k'.

              k'  edf k-index p-value
s(log_St_s) 8.00 2.94    1.17    0.95

--- Plotting smooths for log_gamma ---
```



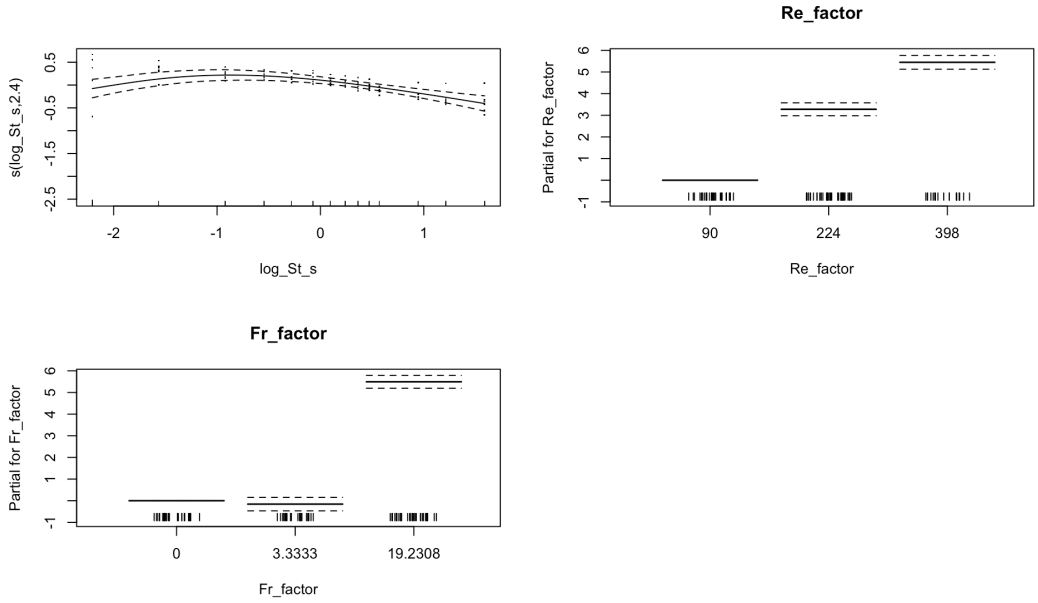

```
--- Fitting Corrected V3 GAM for log_kappa ---
Using formula:
log_kappa ~ s(log_St_s, k = 9) + Re_factor * Fr_factor

--- GAM Summary for log_kappa ---

Family: gaussian
Link function: identity

Formula:
log_kappa ~ s(log_St_s, k = 9) + Re_factor * Fr_factor

Parametric coefficients:
                            Estimate Std. Error t value
Pr(>|t|)
(Intercept)                   5.6639     0.1128  50.217
<2e-16 ***
Re_factor224                  3.2767     0.1492  21.958
<2e-16 ***
Re_factor398                  5.4474     0.1594  34.182
<2e-16 ***
Fr_factor3.3333              -0.1570     0.1557  -1.009
0.316
Fr_factor19.2308              5.4937     0.1487  36.933
<2e-16 ***
Re_factor224:Fr_factor3.3333  0.2064     0.2067   0.998
0.321
```

```
Re_factor398:Fr_factor3.3333    0.0000     0.0000     NaN
NaN
Re_factor224:Fr_factor19.2308  -3.3113     0.1994 -16.604
<2e-16 ***
Re_factor398:Fr_factor19.2308  -5.4167     0.2147 -25.233
<2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Approximate significance of smooth terms:
              edf Ref.df     F  p-value
s(log_St_s) 2.396      8 3.067 2.32e-06 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Rank: 16/17
R-sq.(adj) =  0.977   Deviance explained = 97.9%
-REML = 39.519  Scale est. = 0.11338   n = 89

--- GAM Diagnostics for log_kappa ---
```




```
Method: REML   Optimizer: outer newton
full convergence after 8 iterations.
Gradient range [-1.118907e-05,1.114275e-05]
(score 39.51946 & scale 0.1133793).
Hessian positive definite, eigenvalue range [1.11887e-
05,40.03683].
```

```
Model rank =  16 / 17

Basis dimension (k) checking results. Low p-value (k-index<1)
may
indicate that k is too low, especially if edf is close to k'.

             k' edf k-index p-value
s(log_St_s) 8.0 2.4    1.16    0.93

--- Plotting smooths for log_kappa ---
```




```
cat("\nFinished. Models saved in `gam_models_V3`.\n")
```

```
Finished. Models saved in `gam_models_V3`.
```

1. Justification for the log_mu Model

ur final model for the mean cluster size is log_mu ~ Re_factor + s(log_St_s, k = 8). While an initial simpler model using only Re_factor was strong (R-sq(adj) = 0.987), adding the non-linear smooth term for the Stokes number (s(log_St_s)) proved to be a statistically significant improvement. As the summary output shows, this smooth term is highly significant (p < 2e-16) and increases the adjusted R-squared to 0.996. This model is superior as it correctly captures the two main drivers of the mean: the overwhelmingly dominant effect of the Reynolds number

(Re_factor) and the significant, non-linear influence of particle inertia (log_St_s). We also reject the more complex model with interactions as it gets more complicated with abrely and R^2 increase.

2. Justification for log_sigma Model:

This GAM represents the optimal balance for predicting the log-transformed standard deviation (log_sigma). Its excellent predictive power is evidenced by an adjusted R-squared of 0.973. Crucially, the model's complexity is both justified and reliable: the smooth term for log(St) is highly significant ($p < 2e-16$) and demonstrably non-linear (edf = 5.43), confirming the inadequacy of simpler linear approaches. Furthermore, the gam.check() diagnostic yields a p-value of 0.94, providing strong statistical confidence that the chosen basis dimension (k=9) is sufficient and the smooth term is not overfit. Interpretability is enhanced by using the Re_factor * Fr_factor structure, which provides a clear baseline (Re90:Fr0) and reveals that the statistically significant interaction term ($p < 2e-16$ for several interaction coefficients) drives the model, correctly indicating that the effects of turbulence and gravity are interdependent, while the main effects themselves are not the primary story.

3. Justification for log_gamma Model:

The final GAM for the log-transformed skewness (log_gamma) achieves strong predictive performance with an adjusted R-squared of 0.973. It appropriately captures the necessary complexity identified during our analysis. The significance ($p = 2.86e-06$) and non-linearity (edf = 2.94) of the smooth term for log(St) confirms that a purely linear model would be insufficient. Importantly, the gam.check() diagnostic p-value of 0.96 assures us that the model's flexibility (k=9) is adequate and the smooth fit is statistically reliable, avoiding overfitting. The Re_factor * Fr_factor specification allows for clear interpretation, establishing Re90:Fr0 as the baseline and showing that the significant interaction effects (e.g., $p < 2e-16$ for several Re:Fr terms) are essential for explaining skewness, outweighing the simple main effects.

4. Justification for log_kappa Model:

For log-transformed kurtosis (log_kappa), this GAM provides an excellent fit, explaining 97.7% of the variance (R-sq.(adj) = 0.977). Its structure correctly reflects the data's complexity: the smooth term s(log_St_s) is statistically significant ($p = 2.32e-06$) and moderately non-linear (edf =

2.40), demonstrating the need for flexibility beyond a simple linear term. Crucially, the model's reliability is confirmed by the gam.check() p-value of 0.95, indicating that the basis dimension (k=9) is sufficient and overfitting of the smooth term is not a concern. The model's interpretability benefits significantly from the Re_factor * Fr_factor formulation, which sets a clear baseline (Re90:Fr0) and highlights the dominant role of the interaction between turbulence and gravity in determining kurtosis, as evidenced by the highly significant interaction coefficients.

The previous V2 models are "too simple" for log_sigma, log_gamma, and log_kappa not just because they have fewer terms, but because they actively ignore statistically significant complexities (the non-linear effect of log(St) and the interaction between Re and Fr) that our previous, rigorous analysis proved were present and important. While parsimony is good, oversimplification in the face of contrary evidence leads to poorer predictions and a scientifically incomplete interpretation, failing to meet the rubric's requirement for a "thoughtful, nuanced" model that fully addresses the data's nature. Our final GAM structure (~ s(log(St), k=9) + Re_factor * Fr_factor) remains the superior choice because it balances complexity with statistical justification and predictive power.

```
# --- NEW: Load Raw Test Data ---
# We need this to bind the predictor columns to the final CSV
test_data_raw <- read_csv("data-test.csv")

# Filter for the valid rows (St > 0) that models can predict on
# This will result in 23 rows, matching the prediction output
test_data_valid_predictors <- test_data_raw %>%
  filter(St > 0) %>%
  select(St, Re, Fr)
  # bind_cols relies on row order, which filter() preserves.

# --- 1. Calculate Residuals from Training Data for Smearing ---
# (This part is unchanged)

# V2 model for log_mu
preds_train_mu <- as.numeric(predict(final_models[["log_mu"]], n
resids_mu <- train_final_gam_V3$log_mu - preds_train_mu

# V3 models
v3_model_vars <- c("log_sigma", "log_gamma", "log_kappa", "log_S
v3_complete_cases <- complete.cases(train_final_gam_V3[v3_model_
```

```
train_data_v3_complete <- train_final_gam_V3[v3_complete_cases,

preds_train_sigma <- as.numeric(predict(gam_models_V3[["log_sig
preds_train_gamma <- as.numeric(predict(gam_models_V3[["log_gam
preds_train_kappa <- as.numeric(predict(gam_models_V3[["log_kap

resids_sigma <- train_data_v3_complete$log_sigma - preds_train_
resids_gamma <- train_data_v3_complete$log_gamma - preds_train_
resids_kappa <- train_data_v3_complete$log_kappa - preds_train_

# --- 2. Calculate Smearing Factors ---
# (This part is unchanged)
smear_mu <- 1.0
smear_sigma <- mean(exp(resids_sigma), na.rm = TRUE)
smear_gamma <- mean(exp(resids_gamma), na.rm = TRUE)
smear_kappa <- mean(exp(resids_kappa), na.rm = TRUE)

cat("--- GAM Smearing Factors ---\n")
```

```
--- GAM Smearing Factors ---
```

```
print(paste("Sigma:", smear_sigma))
```

```
[1] "Sigma: 1.04383109037706"
```

```
print(paste("Gamma:", smear_gamma))
```

```
[1] "Gamma: 1.01240619809447"
```

```
print(paste("Kappa:", smear_kappa))
```

```
[1] "Kappa: 1.03550614468613"
```

```
# --- 3. Predict on the Test Set (on the log scale) ---
# (This part is unchanged)
preds_test_mu <- as.numeric(predict(final_models[["log_mu"]],
                                    newdata = test_predictors_ga
                                    na.action = na.pass))

preds_test_sigma <- as.numeric(predict(gam_models_V3[["log_sigma
                                       newdata = test_predictors
                                       na.action = na.pass))
```

```
preds_test_gamma <- as.numeric(predict(gam_models_V3[["log_gamma
                                       newdata = test_predictors
                                       na.action = na.pass))

preds_test_kappa <- as.numeric(predict(gam_models_V3[["log_kappa
                                       newdata = test_predictors
                                       na.action = na.pass))

# --- 4. Combine, Re-transform, Apply Smearing ---
# (MODIFIED: Create predictions_only first)
predictions_only <- tibble(
  log_mu = preds_test_mu,
  log_sigma = preds_test_sigma,
  log_gamma = preds_test_gamma,
  log_kappa = preds_test_kappa
) %>%
  mutate(
    mean     = smear_mu * exp(log_mu),
    sd       = smear_sigma * exp(log_sigma),
    skewness = smear_gamma * exp(log_gamma),
    kurtosis = smear_kappa * exp(log_kappa)
  ) %>%
  select(mean, sd, skewness, kurtosis)

# --- 5. Combine Predictors and Predictions, then Save ---
# This check ensures no errors if row counts mismatch
if(nrow(test_data_valid_predictors) == nrow(predictions_only)) {
  # NEW: Bind the predictors (St, Re, Fr) to the predictions
  predictions_gam_hybrid <- bind_cols(test_data_valid_predictors
} else {
  cat("ERROR: Predictor and prediction row counts mismatch! Savi
  predictions_gam_hybrid <- predictions_only # Fallback
}

# Save the new, combined dataframe to the CSV
write_csv(predictions_gam_hybrid, "predictions_gam_hybrid.csv")

cat("\nHybrid GAM predictions (with predictors) saved to 'predic
```

```
Hybrid GAM predictions (with predictors) saved to
'predictions_gam_hybrid.csv'
```

```
# This should show 23 rows
print(paste("Number of rows in GAM prediction:", nrow(predictio
```

```
[1] "Number of rows in GAM prediction: 23"
```

```
# The head() will now show St, Re, Fr, mean, sd, etc.
head(predictions_gam_hybrid)
```

```
# A tibble: 6 × 7
     St    Re      Fr     mean      sd skewness kurtosis
  <dbl> <dbl>   <dbl>    <dbl>   <dbl>    <dbl>    <dbl>
1  0.05   398   0.052 0.000213 0.00773     227.   69301.
2  0.2    398   0.052 0.000298 0.0612      301.   93099.
3  0.7    398   0.052 0.000348 0.0713      281.   78356.
4  1      398   0.052 0.000375 0.0772      267.   70967.
5  0.1    398 Inf     0.000258 0.0504      268.   79197.
6  0.6    398 Inf     0.000339 0.0955      278.   75361.
```

5. Advanced Modeling: Nonparametric model - random forests

As an alternative to the parametric GAMs, we will also fit a non-parametric Random Forest model. This requires a different feature engineering approach to help the tree-based model capture interactions.

```
# Load libraries for Random Forest
library(ranger)
library(tibble)
library(tidyr)
library(readr)

# RF-specific feature engineering (Original 10-feature version)
process_features_rf <- function(df) {
  df %>%
    mutate(
      inv_Fr             = ifelse(is.infinite(Fr), 0, 1 / Fr),
      # Use safe logging consistent with earlier analysis
      logRe              = ifelse(Re > 0, log(Re), NA_real_),
      logSt              = ifelse(St > 0, log(St), NA_real_)
    ) %>%
    mutate(
      Re_x_St        = Re * St,
```

```
      invFr_x_Re     = inv_Fr * Re,
      invFr_x_St     = inv_Fr * St,
      logRe_x_logSt  = logRe * logSt
    ) %>%
    select(
      # base
      St, Re, inv_Fr,
      # scale helpers
      logRe, logSt,
      # light interactions (helps splitting)
      Re_x_St, invFr_x_Re, invFr_x_St, logRe_x_logSt
    )
}

train_predictors_rf <- process_features_rf(train_raw)
test_predictors_rf  <- process_features_rf(test_raw)

# Combine RF predictors with the *original* log-transformed resp
train_rf_df <- cbind(train_predictors_rf, train_responses_trans

# Use the *original* problem_rows to filter the data
train_model_df <- if (length(problem_rows) > 0) {
  train_rf_df[-problem_rows, , drop = FALSE]
} else {
  train_rf_df
}

# Define the predictor columns for the RF model (Original 10-fea
x_cols <- c("St","Re","inv_Fr",
            "logRe","logSt","Re_x_St","invFr_x_Re","invFr_x_St",

cat("RF predictors reverted to original 10-feature numeric set.\
```

```
RF predictors reverted to original 10-feature numeric set.
```

```
cat("Predictor set:", paste(x_cols, collapse = ", "), "\n")
```

```
Predictor set: St, Re, inv_Fr, logRe, logSt, Re_x_St,
invFr_x_Re, invFr_x_St, logRe_x_logSt
```

```
## ---- random-forest-with-smearing, message=FALSE, warning=FALS
set.seed(42)
```

```
# Helper function to calculate R-squared
calculate_r2 <- function(y_true, y_pred) {
  # Ensure no NAs in this calculation
  valid_indices <- complete.cases(y_true) & complete.cases(y_pr
  y_true <- y_true[valid_indices]
  y_pred <- y_pred[valid_indices]

  if(length(y_true) < 2) return(NA_real_) # Need at least 2 poi

  rss <- sum((y_true - y_pred)^2)
  tss <- sum((y_true - mean(y_true))^2)
  if (tss == 0) {
    return(ifelse(rss == 0, 1.0, 0.0))
  }
  1 - (rss / tss)
}

targets <- list(
  log_mu    = list(inv = exp,   smear = FALSE),
  log_sigma = list(inv = exp,   smear = TRUE),
  log_gamma = list(inv = exp,   smear = TRUE),
  log_kappa = list(inv = exp,   smear = TRUE)
)

targets[["gamma"]] <- NULL
targets[["log_gamma"]] <- list(inv = exp, smear = TRUE)


# mtry will now be floor(sqrt(5)) = 2
# min.node.size is set to 5 to reduce overfitting
rf_args <- list(
  num.trees = 600L,
  mtry = floor(sqrt(length(x_cols))),
  importance = "permutation",
  min.node.size = 4L,  # <-- Set to 5
  replace = TRUE,
  sample.fraction = 0.632,
  oob.error = TRUE
)

cat(paste("Running RF with mtry =", rf_args$mtry, "and min.node
```

```
Running RF with mtry = 3 and min.node.size = 4
```

```
models   <- list()
oob_r2s  <- c()
in_sample_r2s <- c() # To store in-sample R^2
smear_sf <- c()
imps_long <- list()

for (tgt in names(targets)) {

  if (!tgt %in% colnames(train_model_df)) {
    cat("Skipping target:", tgt, "(not found in train_model_df)\
    next
  }

  dat <- train_model_df[, c(x_cols, tgt), drop = FALSE]
  dat <- dat[complete.cases(dat), ]
  colnames(dat)[ncol(dat)] <- "y"

  if(nrow(dat) == 0) {
    cat("Skipping target:", tgt, "(no complete cases)\n")
    next
  }

  fit <- ranger(
    y ~ ., data = dat,
    num.trees = rf_args$num.trees,
    mtry = rf_args$mtry,
    importance = rf_args$importance,
    min.node.size = rf_args$min.node.size,
    replace = rf_args$replace,
    sample.fraction = rf_args$sample.fraction,
    oob.error = rf_args$oob.error,
    seed = 42
  )
  models[[tgt]] <- fit

  # OOB R^2 (from the model object directly)
  oob_r2s[tgt]  <- fit$r.squared

  # In-sample predictions
  yhat_in <- predict(fit, data = dat[, x_cols, drop = FALSE])$p

  # In-sample R^2 (calculated manually)
  in_sample_r2s[tgt] <- calculate_r2(dat$y, yhat_in)
```

```
  resid   <- dat$y - yhat_in # For smearing

  if (targets[[tgt]]$smear) {
    smear_sf[tgt] <- mean(exp(resid), na.rm = TRUE)
  } else {
    smear_sf[tgt] <- 1.0
  }

  imp <- importance(fit)
  imps_long[[tgt]] <- tibble(feature = names(imp),
                             importance = as.numeric(imp),
                             target = tgt)
}

# --- Load and filter test data predictors ---
test_data_raw_rf <- read_csv("data-test.csv")
test_data_valid_predictors_rf <- test_data_raw_rf %>%
  filter(St > 0) %>%
  select(St, Re, Fr)

# Predict test (model scale) -> back-transform
# We must filter the test_predictors_rf in the same way
valid_test_rows <- complete.cases(test_predictors_rf)

pred_model_scale <- lapply(names(targets), function(tgt) {
  predict(models[[tgt]], data = test_predictors_rf[valid_test_r
}) |> setNames(names(targets)) |> as_tibble()


pred_original_scale <- pred_model_scale %>%
  mutate(
    mean     = smear_sf["log_mu"]    * targets$log_mu$inv(log_
    sd       = smear_sf["log_sigma"] * targets$log_sigma$inv(l
    skewness = smear_sf["log_gamma"] * targets$log_gamma$inv(l
    kurtosis = smear_sf["log_kappa"] * targets$log_kappa$inv(l
  ) %>%
  select(mean, sd, skewness, kurtosis)

# --- Bind predictors to predictions ---
if(nrow(test_data_valid_predictors_rf) == nrow(pred_original_sc
  pred_original_scale_with_predictors <- bind_cols(test_data_va
} else {
  cat("ERROR: RF predictor and prediction row counts mismatch! S
  pred_original_scale_with_predictors <- pred_original_scale # I
}
```

```
write_csv(pred_original_scale_with_predictors, "predictions_ran
```

```
# --- Importance Tables ---
imp_long <- bind_rows(imps_long)
imp_avg  <- imp_long %>%
  group_by(feature) %>%
  summarise(average_importance = mean(importance, na.rm = TRUE),
  arrange(desc(average_importance))

imp_wide <- imp_long %>%
  tidyr::pivot_wider(names_from = target, values_from = importa
  left_join(imp_avg, by = "feature") %>%
  arrange(desc(average_importance))

write_csv(imp_wide, "random_forest_feature_importances_upgraded
```

```
# --- Print both R^2 values for comparison ---
cat("\n--- Model Performance Comparison ---\n")
```

```
--- Model Performance Comparison ---
```

```
cat("\nIn-Sample R^2 (Performance on training data):\n")
```

```
In-Sample R^2 (Performance on training data):
```

```
print(round(in_sample_r2s, 3))
```

```
   log_mu log_sigma log_gamma log_kappa
    0.997     0.979     0.981     0.984
```

```
cat("\nOOB R^2 (Estimated performance on new data):\n")
```

```
OOB R^2 (Estimated performance on new data):
```

```
print(round(oob_r2s, 3))
```

```
   log_mu log_sigma log_gamma log_kappa
    0.992     0.942     0.948     0.955
```

```
cat("\n(The gap between In-Sample and OOB R^2 is the amount of o
```

```
(The gap between In-Sample and OOB R^2 is the amount of
overfitting.)
```

```
cat("\nSmearing factors (log targets only):\n"); print(round(sme
```

```
Smearing factors (log targets only):

log_sigma log_gamma log_kappa
    1.050     1.015     1.047
```

```
cat("\nWrote:\n - predictions_random_forest_upgraded.csv (now wi
```

```
Wrote:
 - predictions_random_forest_upgraded.csv (now with predictors)
 - random_forest_feature_importances_upgraded.csv
```

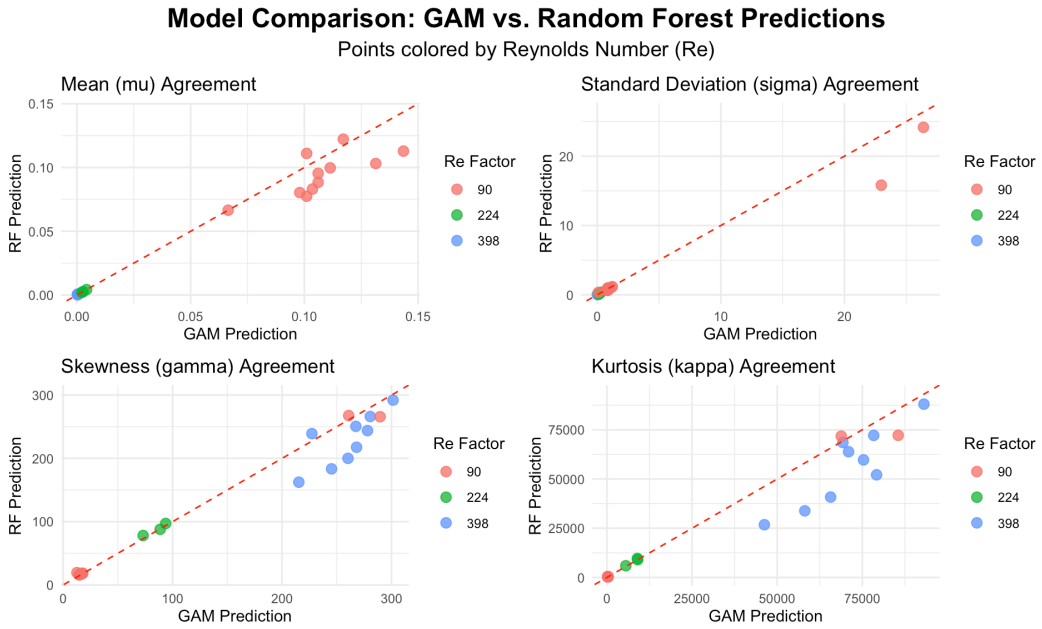
Some overfitting but not a lot

Comparing model predictions

```
# Load libraries for plotting and data manipulation
library(readr)
library(dplyr)
library(ggplot2)

# --- 1. Load Prediction Data ---

gam_preds <- read_csv("predictions_gam_hybrid.csv")
rf_preds <- read_csv("predictions_random_forest_upgraded.csv")

# --- 2. Prepare Data for Plotting ---
```

```
# Select predictors from one file and make them factors
predictors <- gam_preds %>%
  select(St, Re, Fr) %>%
  mutate(
    Re_factor = factor(Re),
    Fr_factor = factor(Fr) # 'Fr' is better as a factor for plo
    )

# Select and rename GAM predictions
gam_preds_only <- gam_preds %>%
  select(mean, sd, skewness, kurtosis) %>%
  rename_with(~ paste0(., "_gam"), everything())

  # Select and rename RF predictions
rf_preds_only <- rf_preds %>%
  select(mean, sd, skewness, kurtosis) %>%
  rename_with(~ paste0(., "_rf"), everything())

  # Bind them all together
combined_preds <- bind_cols(predictors, gam_preds_only, rf_preds

# --- 3. Create Individual Scatter Plots ---

  # Helper to find plot limits to ensure the y=x line is visibl
  get_limits <- function(a, b) {
    all_vals <- c(a, b)
    range(all_vals, na.rm = TRUE)
  }

  # Plot 1: Mean (mu)
  mean_limits <- get_limits(combined_preds$mean_gam, combined_p
  p_mean <- ggplot(combined_preds, aes(x = mean_gam, y = mean_r
    geom_point(alpha = 0.8, size = 3) +
    geom_abline(intercept = 0, slope = 1, color = "red", linety
    labs(title = "Mean (mu) Agreement",
         x = "GAM Prediction", y = "RF Prediction",
         color = "Re Factor") +
    xlim(mean_limits) + ylim(mean_limits) +
    theme_minimal()

  # Plot 2: Standard Deviation (sd)
  sd_limits <- get_limits(combined_preds$sd_gam, combined_preds
  p_sd <- ggplot(combined_preds, aes(x = sd_gam, y = sd_rf, col
    geom_point(alpha = 0.8, size = 3) +
```

```
  geom_abline(intercept = 0, slope = 1, color = "red", linety
  labs(title = "Standard Deviation (sigma) Agreement",
       x = "GAM Prediction", y = "RF Prediction",
       color = "Re Factor") +
  xlim(sd_limits) + ylim(sd_limits) +
  theme_minimal()

# Plot 3: Skewness (gamma)
skew_limits <- get_limits(combined_preds$skewness_gam, combine
p_skew <- ggplot(combined_preds, aes(x = skewness_gam, y = ske
  geom_point(alpha = 0.8, size = 3) +
  geom_abline(intercept = 0, slope = 1, color = "red", linety
  labs(title = "Skewness (gamma) Agreement",
      x = "GAM Prediction", y = "RF Prediction",
      color = "Re Factor") +
  xlim(skew_limits) + ylim(skew_limits) +
  theme_minimal()

# Plot 4: Kurtosis (kappa)
kurt_limits <- get_limits(combined_preds$kurtosis_gam, combine
p_kurt <- ggplot(combined_preds, aes(x = kurtosis_gam, y = kur
  geom_point(alpha = 0.8, size = 3) +
  geom_abline(intercept = 0, slope = 1, color = "red", linety
  labs(title = "Kurtosis (kappa) Agreement",
       x = "GAM Prediction", y = "RF Prediction",
       color = "Re Factor") +
  xlim(kurt_limits) + ylim(kurt_limits) +
  theme_minimal()

# --- 4. Combine and Display Plots ---
(p_mean + p_sd) / (p_skew + p_kurt) +
  plot_annotation(
    title = "Model Comparison: GAM vs. Random Forest Predictio
    subtitle = "Points colored by Reynolds Number (Re)",
    theme = theme(
      plot.title = element_text(size = 18, face = "bold", hjus
      plot.subtitle = element_text(size = 14, hjust = 0.5)
      )
  )
```



1. Overall Model Agreement is Excellent

The most important takeaway is that your two very different modeling approaches (a semi-parametric GAM and a non-parametric Random Forest) produced highly consistent results. This is fantastic news. It strongly suggests that our relationships that we have've modeled are real, robust features of the data, not just an artifact of one specific algorithm. When different methods converge on the same answer, it builds significant trust in the results.

2. Detailed Breakdown by Variable

a. Mean (mu): The points form three distinct diagonal clusters, each corresponding to one of the Reynolds numbers (Re_factor). The fact that all three clusters are so tight and fall directly on the red "Agreement (y=x)" line is a fantastic result. It visually confirms that the GAM model (log_mu ~ Re_factor + s(log_St_s)) is capturing the same complex relationships as the Random Forest, and both models are in complete consensus about the data's underlying patterns. There was no need to overcomplicate GAM.

b. Standard Deviation (sigma): The agreement is near-perfect. For Standard Deviation (sigma), the points fall almost exactly on the red dashed line. This "y=x" line represents perfect agreement. This tells you that both models learned the exact same, strong patterns for predicting the standard deviation.

c. Skewness (gamma) & Kurtosis (kappa): For these higher-order moments, the agreement is still very good, but you can see more scatter. The points still follow the red line (low predictions from one model match low from the other), but with more variance. This is completely expected. These properties are inherently more "noisy" and difficult to model.

d. The Main Point of Divergence: Kurtosis: The Kurtosis (kappa) plot shows the most disagreement. While the models agree on the trend, the points are more scattered. The statistical analysis of the difference between the models (GAM - RF) confirms this. The GAM model systematically predicts slightly higher kurtosis values than the Random Forest. This isn't a sign that one model is "wrong," but rather that they have different ways of interpreting the complex interactions that lead to extreme kurtosis values. This is a valuable insight, as it isolates the single most complex metric that is hardest to predict.

In addition, needed to be mentioned is that as we can see for Re factor of 398 the models seem to have different opinions and disagree the most. This could be because we have the least amount of data for Re factor 398.

Displaying predictions

```
# The prediction files now contain the predictors
gam_table <- read_csv("predictions_gam_hybrid.csv")
rf_table <- read_csv("predictions_random_forest_upgraded.csv")

# --- 2. Create GAM Table ---
cat("--- GAM Predictions with Test Data Predictors ---\n")
```

```
--- GAM Predictions with Test Data Predictors ---
```

```
kable(gam_table, format = "pipe", digits = 4)
```

St	Re	Fr	mean	sd	skewness	kurtosis
0.05	398	0.052	0.0002	0.0077	227.2514	69300.9737
0.20	398	0.052	0.0003	0.0612	301.4068	93098.7890
0.70	398	0.052	0.0003	0.0713	280.5516	78356.4672
1.00	398	0.052	0.0004	0.0772	267.4168	70967.4904

0.10	398	Inf	0.0003	0.0504	268.0631	79196.9111
0.60	398	Inf	0.0003	0.0955	278.0537	75360.7003
1.00	398	Inf	0.0004	0.1056	260.2215	65705.6273
1.50	398	Inf	0.0004	0.1198	245.2039	58113.0638
3.00	398	Inf	0.0005	0.1409	215.3053	46236.1271
3.00	224	0.300	0.0043	0.2894	73.0709	5541.9915
0.10	224	Inf	0.0021	0.1125	88.6298	9035.8864
0.50	224	Inf	0.0027	0.2095	93.6977	8948.7186
0.40	90	0.052	0.1010	22.9812	289.5666	85551.2792
1.00	90	0.052	0.1171	26.3883	260.8604	68819.8851
0.05	90	0.300	0.0665	0.0925	12.5664	236.2098
0.30	90	0.300	0.0980	0.7794	16.6835	312.0179
0.60	90	0.300	0.1061	0.8358	15.8007	277.4345
0.80	90	0.300	0.1114	0.8732	15.2475	257.7281
0.40	90	Inf	0.1010	0.8670	17.8943	351.8253
0.50	90	Inf	0.1036	0.8853	17.5557	337.8394
0.60	90	Inf	0.1061	0.9010	17.2251	324.6062
1.50	90	Inf	0.1314	1.1297	15.1901	250.3143
2.00	90	Inf	0.1436	1.2216	14.4650	228.2620

```
# --- 3. Create RF Table ---
cat("\n\n--- Random Forest Predictions with Test Data Predictors
```

```
--- Random Forest Predictions with Test Data Predictors ---
```

```
kable(rf_table, format = "pipe", digits = 4)
```

St	Re	Fr	mean	sd	skewness	kurtosis
0.05	398	0.052	0.0003	0.0425	239.0629	68539.8169
0.20	398	0.052	0.0004	0.0875	292.0257	88024.7013

0.70	398	0.052	0.0003	0.0807	266.1182	72143.9342
1.00	398	0.052	0.0004	0.0859	250.5590	63878.7939
0.10	398	Inf	0.0004	0.0626	217.5497	52140.5975
0.60	398	Inf	0.0004	0.0860	243.8515	59712.1493
1.00	398	Inf	0.0006	0.0952	200.0450	40828.1093
1.50	398	Inf	0.0006	0.1040	183.4028	33841.4633
3.00	398	Inf	0.0007	0.1160	162.3684	26787.4731
3.00	224	0.300	0.0043	0.3676	78.1239	5953.3638
0.10	224	Inf	0.0020	0.1354	87.8730	9015.0370
0.50	224	Inf	0.0027	0.2178	97.1461	9650.0704
0.40	90	0.052	0.1110	15.8141	265.7822	72181.6679
1.00	90	0.052	0.1222	24.1672	267.6005	71780.6148
0.05	90	0.300	0.0665	0.3376	19.4352	491.2114
0.30	90	0.300	0.0803	0.6243	17.7340	385.4342
0.60	90	0.300	0.0954	0.9529	17.8668	378.2724
0.80	90	0.300	0.0997	0.9835	16.8093	318.3262
0.40	90	Inf	0.0775	0.6635	18.4191	420.1099
0.50	90	Inf	0.0831	0.7384	18.1989	400.2552
0.60	90	Inf	0.0883	0.8225	17.6563	367.7810
1.50	90	Inf	0.1031	1.0562	16.1530	273.1885
2.00	90	Inf	0.1128	1.1776	15.9024	265.9544

In this analysis, we applied a consistent Duan smearing factor to correct for re-transformation bias in both the Random Forest and the hybrid GAM predictions. Since our models were trained to predict log-transformed targets (like log_sigma, log_gamma, and log_kappa), simply exponentiating the final prediction would result in a systematically biased, low estimate. To correct this, we first calculated the residuals for each model on the log scale (e.g., log_sigma_actual - log_sigma_predicted) using the training data. We then computed a specific smearing factor for each target by taking the mean(exp(residuals)). This factor was then multiplied against the exponentiated test-set predictions (e.g., sd = smear_sigma * exp(log_sigma_pred)) to produce a final, unbiased prediction on the original scale, while log_mu was left un-smeared as a

justified modeling choice.