# Case Study: Modeling Liquid Mechanics

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## Introduction

Our key research objectives include understanding and predicting how turbulence affects the dynamics of water droplets and ice crystals (how they collide and mix) in clouds. With our machine learning model, we are trying to infer the volume distribution of clusters within clouds.

To do this, we began by doing some basic Exploratory Data Analysis on the three predictor variables: Reynolds number (`Re`), gravitational acceleration (`Fr`), and particle characteristic (`St`). (Our graphs are included in Appendix: Section 1)

## Methodology

```
head(train)
```

```
##     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
```

```
train_data <- train %>%
  mutate(Fr = as.ordered(Fr)) %>%
  mutate(Re = as.ordered(Re))
```

We decided at the beginning to treat Fr and Re as ordered factors. It makes sense to treat Fr as a categorical variable because we are given only three unique values, one of which is infinity, and in practice the three values are representative of different types of clouds. We decided to treat Re as a factored variable as well because we are also only given three unique values and because the differences between the three values are so large that it would be unwise to extrapolate our model to the ranges in between the values we are given. In terms of prediction and inference, we believe our models can still be generalized to Fr and Re values similar to the ones we are working with.

```
first_lm_R1 <- lm(R_moment_1 ~ St + Re + Fr, data = train_data)
first_lm_R2 <- lm(R_moment_2 ~ St + Re + Fr, data = train_data)
first_lm_R3 <- lm(R_moment_3 ~ St + Re + Fr, data = train_data)
first_lm_R4 <- lm(R_moment_4 ~ St + Re + Fr, data = train_data)
summary(first_lm_R1)$r.squared
```

```
## [1] 0.9293093
```

```
summary(first_lm_R4)$r.squared
```

```
## [1] 0.4252642
```

We decided to initially fit the most basic linear model with all three predictors to see what it would look like. The model for the first moment had a fairly high $R^2$ value (0.929), but the model for the fourth moment had a much lower $R^2$ value (0.425). Additionally, in our diagnostic plots (see Appendix: Section 2), we saw a pattern in the residuals vs fitted values plots where the models would consistently under predict in some areas and over predict in others, indicating non-linearity. In addition, looking at the Normal Q-Q plots, the normality assumption also seemed to be violated for higher moments. This is consistent with the fact that our histogram of St in our EDA was not normally distributed.

This information lead us to try using a GAM to model the relationship between the predictors and the 4 moments due to the increased flexbility GAMs provide. However, we knew that using GAMs made interpretability an issue, because interpreting a complex smooth function of a continuous predictor is very hard.

As a result, we decided to use variable transformations and interaction effects to make linear models with suitable model diagnostics for all 4 moments for the purpose of inference. We also tried doing forward selection with AIC to see if we could select a simpler model in case were overfitting, but our resulting models were the same as our input models (see Appendix: Section 2). We chose AIC over BIC because we assume that fluid mechanics is a complex process to model, therefore parity is not expected. We would also compare our final linear models with 4 GAM models (one for each moment) using 10-fold CV in order to find the best models for prediction.

## Results

### Final Linear Model

```r
lm1 <- lm(log(R_moment_1) ~ log(St) + Re + Fr + St*Fr + Fr*Re + St*Re, data = train_data)
summary(lm1)
```

```
##
## Call:
## lm(formula = log(R_moment_1) ~ log(St) + Re + Fr + St * Fr +
##     Fr * Re + St * Re, data = train_data)
##
## Residuals:
##       Min        1Q    Median        3Q       Max
## -0.211809 -0.042926 -0.006391  0.038831  0.171243
##
## Coefficients: (1 not defined because of singularities)
##              Estimate Std. Error  t value Pr(>|t|)
## (Intercept) -5.349488   0.027649 -193.480  < 2e-16 ***
## log(St)      0.145668   0.014562   10.003 1.89e-15 ***
## Re.L        -4.028476   0.027949 -144.139  < 2e-16 ***
## Re.Q         0.644476   0.022457   28.698  < 2e-16 ***
## Fr.L        -0.102135   0.019793   -5.160 1.95e-06 ***
## Fr.Q         0.109493   0.026874    4.074 0.000113 ***
## St           0.095896   0.021136    4.537 2.13e-05 ***
## Fr.L:St      0.095376   0.017271    5.522 4.60e-07 ***
## Fr.Q:St     -0.064244   0.022042   -2.915 0.004692 **
## Re.L:Fr.L    0.242947   0.024770    9.808 4.39e-15 ***
## Re.Q:Fr.L   -0.076314   0.022588   -3.379 0.001159 **
## Re.L:Fr.Q   -0.077781   0.046306   -1.680 0.097169 .
## Re.Q:Fr.Q          NA         NA       NA       NA
## Re.L:St     -0.008897   0.021672   -0.411 0.682581
## Re.Q:St     -0.025325   0.018376   -1.378 0.172252
## ---
```

```
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.07645 on 75 degrees of freedom
## Multiple R-squared:  0.999,  Adjusted R-squared:  0.9988
## F-statistic:  5797 on 13 and 75 DF,  p-value: < 2.2e-16
```

```
(lm2 <- lm(log(R_moment_2) ~ log(St) + Re + Fr + St*Fr + Fr*Re + St*Re, data = train_data))
```

```
##
## Call:
## lm(formula = log(R_moment_2) ~ log(St) + Re + Fr + St * Fr +
##     Fr * Re + St * Re, data = train_data)
##
## Coefficients:
## (Intercept)      log(St)         Re.L         Re.Q         Fr.L         Fr.Q
##   -0.300240     1.500864    -4.269814     1.098368    -1.927717     0.946857
##          St     Fr.L:St      Fr.Q:St    Re.L:Fr.L    Re.Q:Fr.L    Re.L:Fr.Q
##   -0.997463    -0.007867    -0.043393     3.399373    -0.646249    -2.588037
##   Re.Q:Fr.Q     Re.L:St      Re.Q:St
##          NA    -0.470624    -0.128587
```

```
summary(lm2)$r.squared
```

```
## [1] 0.955342
```

```
(lm3 <- lm(log(R_moment_3) ~ log(St) + Re + Fr + St*Fr + Fr*Re + St*Re, data = train_data))
```

```
##
## Call:
## lm(formula = log(R_moment_3) ~ log(St) + Re + Fr + St * Fr +
##     Fr * Re + St * Re, data = train_data)
##
## Coefficients:
## (Intercept)      log(St)         Re.L         Re.Q         Fr.L         Fr.Q
##     4.54701      2.36189     -4.89792      1.52364     -3.75114      1.83513
##          St      Fr.L:St      Fr.Q:St    Re.L:Fr.L    Re.Q:Fr.L    Re.L:Fr.Q
##    -1.72871     -0.09194     -0.03580      6.45803     -1.15825     -4.96308
##   Re.Q:Fr.Q      Re.L:St      Re.Q:St
##          NA     -0.79750     -0.17827
```

```
summary(lm3)$r.squared
```

```
## [1] 0.9458698
```

```
(lm4 <- lm(log(R_moment_4) ~ log(St) + Re + Fr + St*Fr + Fr*Re + St*Re, data = train_data))
```

```
##
## Call:
## lm(formula = log(R_moment_4) ~ log(St) + Re + Fr + St * Fr +
##     Fr * Re + St * Re, data = train_data)
##
## Coefficients:
## (Intercept)      log(St)         Re.L         Re.Q         Fr.L         Fr.Q
##     9.28287      3.10948     -5.63270      1.94835     -5.55550      2.71540
##          St      Fr.L:St      Fr.Q:St    Re.L:Fr.L    Re.Q:Fr.L    Re.L:Fr.Q
##    -2.36662     -0.17635     -0.01987      9.47956     -1.66019     -7.28081
##   Re.Q:Fr.Q      Re.L:St      Re.Q:St
##          NA     -1.08269     -0.22245
```

```r
summary(lm4)$r.squared
```

```
## [1] 0.9457368
```

All three of our main predictors: Fr, St, and Re, seem to be significant predictors of the R moments. A one percent increase in Stokes number is associated with 0.146% increase in R moment 1, holding all other predictors constant. When the Reynolds number is 224, the R moment 1 is expected to decrease by 403% from when the Reynolds number is 90, holding all other predictors constant. When the Reynolds number is 398, the R moment 1 is expected to increase by 64% compared to when the Reynolds number is 90.

The interaction terms Fr*St and Re*Fr seem to be significant as well. This is consistent with what we expected from our EDA. When Fr is 0.3, the relationship between R moment 1 and St is positive, however, when Fr is infinity, the relationship between R moment 1 and St is negative. Additionally, we see that when the Froud number is 0.3 and the Reynolds number is 224, the R moment 1 is expected to be an additional 24% lower compared to when either of those conditions are not met.

What these results mean for the research question is that Reynolds number (`Re`), gravitational acceleration (`Fr`), and particle characteristic (`St`) all predict cluster formation in clouds to some degree, even after accounting for the effects of each of the other variables. We can also conclude that direction of the relationship between cluster density and Stokes number is different based on what the Froud number is.

**Predicted Test Error For R Moments 1-4 With Linear Model**
Predicted Mean-Squared Error For R Moment 1

```
## [1] 2.864351e-05
```

Predicted Mean-Squared Error For R Moment 2

```
## [1] 4621.783
```

Predicted Mean-Squared Error For R Moment 3

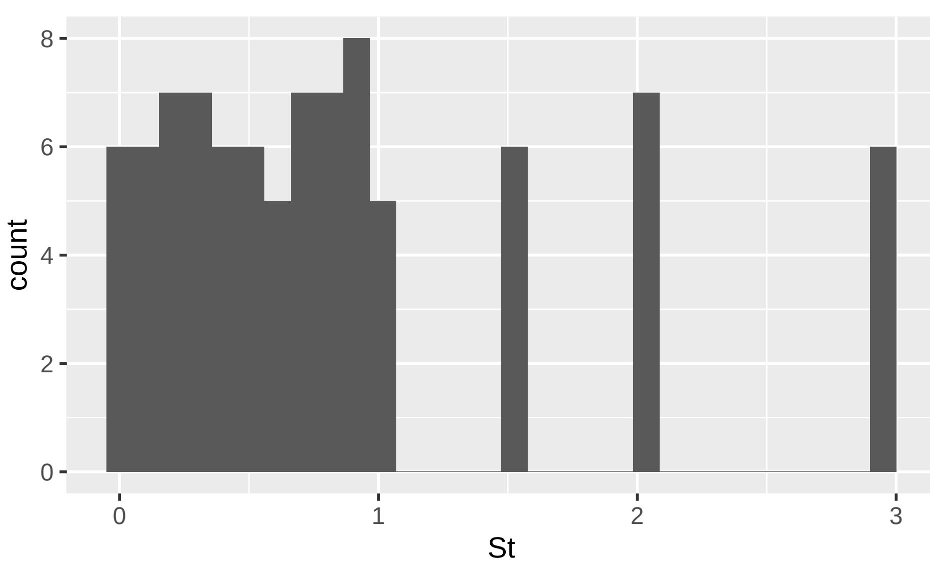
```
## [1] 578718160228
```

Predicted Mean-Squared Error For R Moment 4

```
## [1] 5.488601e+19
```

## Appendix

**Figure 1.1: Distribution of St**



We will try using a log transform on the St variable since the distribution for the St variable is not normally distributed.

**Figure 1.2: R Moments and Re Colored by Fr**

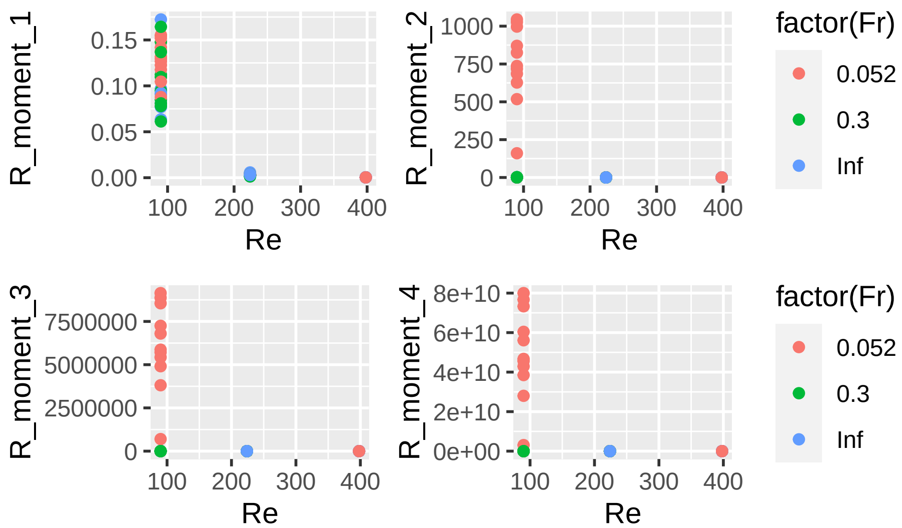
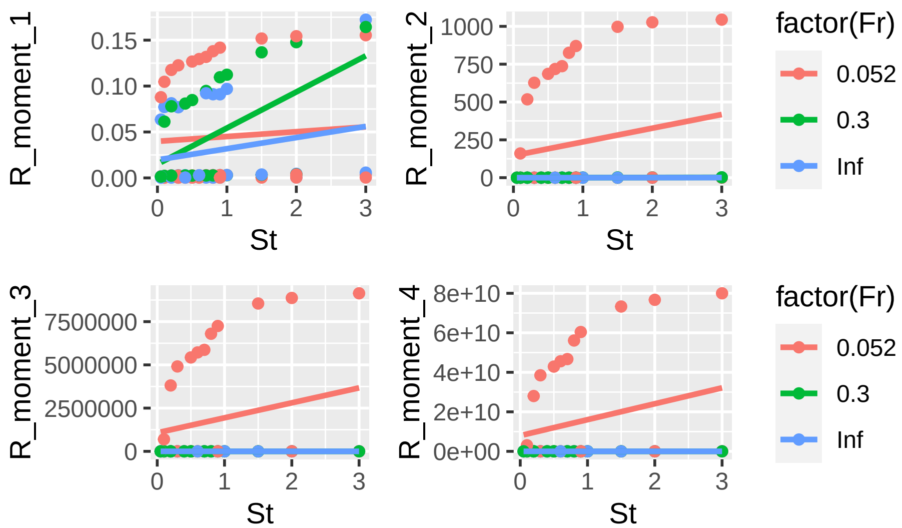
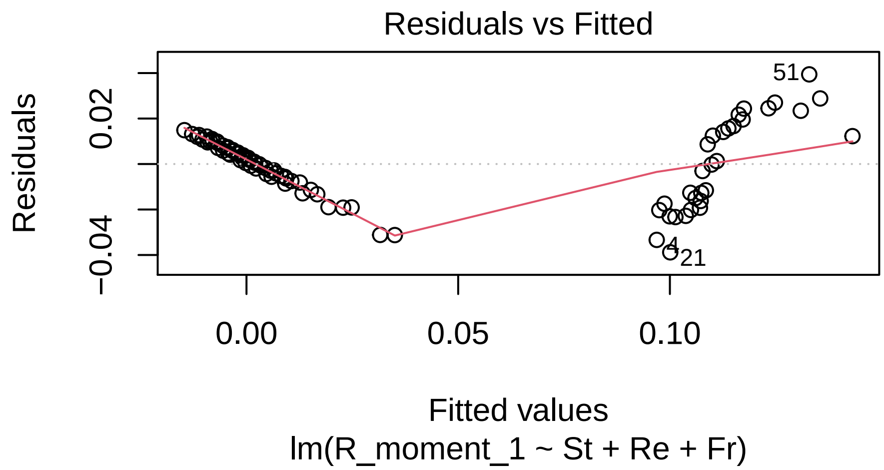



**Figure 1.3: R Moments and St Colored by Fr**




The graphs above show some evidence of interactions, so we will explore interaction terms in our model.

**Figure 2.1-2: Diagnostic Plots For Inital Linear Model of R Moment 1**



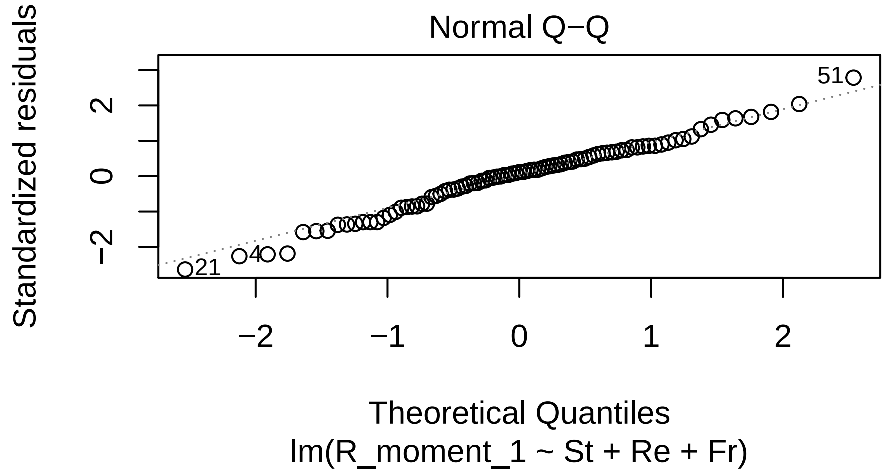
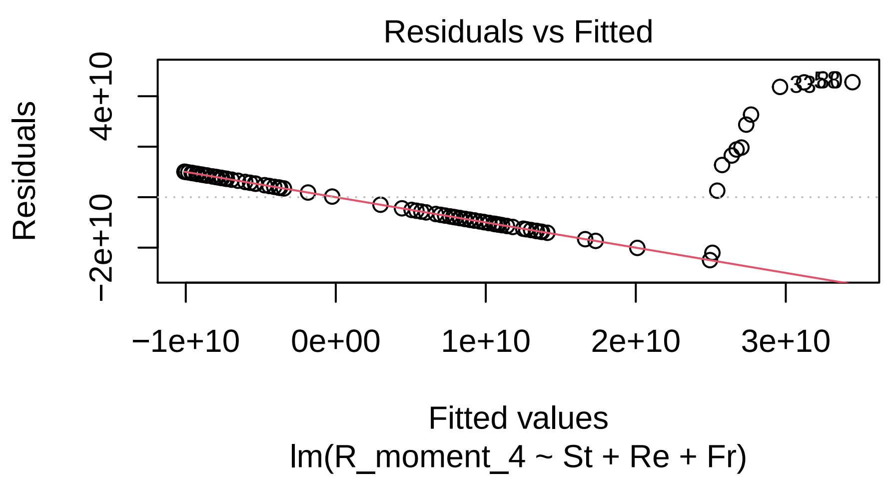
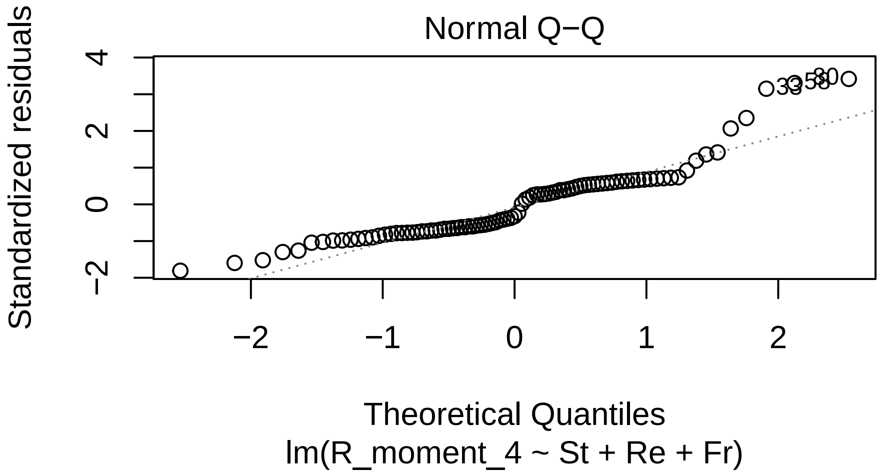




**Figure 2.3-4: Diagnostic Plots For Inital Linear Model of R Moment 4**






Because the linearity condition is not fulfilled in the above Residuals vs. Fitted plots, we will consider performing a log transformation on our response variables (R moments 1-4).

**Figure 2.5: Forward Selection With AIC On Linear Models**

```r
lm1 <- lm(log(R_moment_1) ~ log(St) + Re + Fr + St*Fr + Fr*Re + St*Re, data = train_data)
step(lm1, direction = "forward")
```

```
## Start:  AIC=-444.89
## log(R_moment_1) ~ log(St) + Re + Fr + St * Fr + Fr * Re + St *
##     Re

##
## Call:
## lm(formula = log(R_moment_1) ~ log(St) + Re + Fr + St * Fr +
##     Fr * Re + St * Re, data = train_data)
##
## Coefficients:
## (Intercept)      log(St)         Re.L         Re.Q         Fr.L         Fr.Q
##   -5.349488     0.145668    -4.028476     0.644476    -0.102135     0.109493
##          St     Fr.L:St      Fr.Q:St    Re.L:Fr.L    Re.Q:Fr.L    Re.L:Fr.Q
##    0.095896     0.095376    -0.064244     0.242947    -0.076314    -0.077781
##   Re.Q:Fr.Q      Re.L:St      Re.Q:St
##          NA    -0.008897    -0.025325
```

```r
lm2 <- lm(log(R_moment_2) ~ log(St) + Re + Fr + St*Fr + Fr*Re + St*Re, data = train_data)
#step(lm2, direction = "forward")

lm3 <- lm(log(R_moment_3) ~ log(St) + Re + Fr + St*Fr + Fr*Re + St*Re, data = train_data)
#step(lm3, direction = "forward")

lm4 <- lm(log(R_moment_4) ~ log(St) + Re + Fr + St*Fr + Fr*Re + St*Re, data = train_data)
step(lm4, direction = "forward")
```

```
## Start:  AIC=131.52
## log(R_moment_4) ~ log(St) + Re + Fr + St * Fr + Fr * Re + St *
##     Re

##
## Call:
```

```
## lm(formula = log(R_moment_4) ~ log(St) + Re + Fr + St * Fr +
##     Fr * Re + St * Re, data = train_data)
##
## Coefficients:
## (Intercept)      log(St)         Re.L         Re.Q         Fr.L         Fr.Q
##     9.28287      3.10948     -5.63270      1.94835     -5.55550      2.71540
##          St      Fr.L:St      Fr.Q:St    Re.L:Fr.L    Re.Q:Fr.L    Re.L:Fr.Q
##    -2.36662     -0.17635     -0.01987      9.47956     -1.66019     -7.28081
##   Re.Q:Fr.Q      Re.L:St      Re.Q:St
##          NA     -1.08269     -0.22245
```