Case Report

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1 Introduction

Turbulence is a fundamental concept in fluid mechanics. Understanding how fluids move has enormous importance to a vast range of problems, with practical applications in aeronautical engineering, environmental science, astronomy, and more. In contrast to laminar flow, turbulent flow is irregular, unpredictable, and energy-dissipating. Turbulence enhances mixing which leads to non-uniform distribution of particles and cluster formation. In general, the final state of particles subject to turbulent flow is determined by three main parameters: Reynolds (Re) number, Froude (Fr) number and Stokes (St) number. The Reynolds number is a measure of the intensity of turbulence, with a higher Reynolds number corresponding to a higher intensity of turbulence (J. den Toonder et al., 1997). Broadly speaking, a Reynolds number > 4000 generally represents a relatively chaotic and turbulent flow, a Reynolds number < 2300 generally represents a smooth laminar flow and any number in between typically represents transient flow (Schlichting et al., 2017). The Froude number is a measure of the impact of gravitational acceleration on fluid motion. For instance, a cumulonimbus cloud at a high level above the ground will have a smaller Froude number (compared to lower hanging stratus clouds) because it experiences a lower intensity of gravitational acceleration relative to other clouds (Chanson, 2009). Stokes number is a description of particle properties; a large Stokes number correlates with large particle size which tends to form relatively loose clusters (Ireland et al., 2016).

Despite the importance of turbulence and particle clustering, we do not understand this process well very. Researchers has primarily used Direct Numerical Simulation (DNS) of Navier-Stokes equations to study this problem, but it is extremely time consuming and computationally expensive (Moin & Mahesh, 1998). In addition, the DNS method cannot be practically applied to simulate flows with large Reynolds numbers which requires high resolution, leading to long computation time. However, large Reynolds numbers is highly relevant to real life situations (atmospheric, oceanic turbulence flow). Thus, the primary research **objective** of this study is to build a statistical model to investigate how Reynolds (Re) number, Froude (Fr) number and Stokes (St) number influence particle cluster volume distribution and allows prediction without the need for simulation.

The data for this study comes from Direct Numerical Simulation using a range of parameters. Then, Voronoi Tessellation, a technique that looks at general features of individual clusters in the underlying turbulence, has been applied to generate a distribution of cluster volumes. Since this probability distribution of cluster volumes is harder for statistical learning methods to work with, we will summarize this distribution by its first four raw moments $E(X)$, $E(X^2)$, $E(X^3)$, and $E(X^4)$, the latter three which we transform to central moments as response variables for inference and back for prediction. Theoretically, we are interested in the insights for each of these four moments - the mean of the distribution could be a good indicator of how flow behaves on average, the variance of the distribution could dictate how flow varies over time, the skew of the distribution could illustrate asymmetric properties of the flow, and the kurtosis of the distribution could indicate how particular cluster volumes deviate. We hope that our research model will enable a quick and efficient prediction of a particle cluster volume distribution and enhance our understanding of the relative influence of these parameters in turbulent flow.

2 Methods

2.1 Model

The forms of the statistical models, one for each moment, are:

$$R\_moment_1 \sim Fr + Re + St * (Fr, Re)$$

$$central_2 \sim Fr + Re + poly(St^{1/4}, 2) * (Fr, Re)$$
$$central_3 \sim Fr + Re + poly(St^{1/3}, 2) * (Fr, Re)$$
$$central_4 \sim Fr + Re + poly(\sqrt{St}, 2) * (Fr, Re)$$

where $Fr \in \{0.052, 0.3, \inf\}$ and $Re \in \{90, 224, 398\}$ are categorical variables and (Fr, Re) is an interaction term with 9 levels representing all combinations of Fr and Re. For the fitted coefficients, see the results section.

2.2 Justification

While Fr and Re are continuous values in physics, both variables contain only three levels in our training and test data (Appendix). Since we see from the test data that we are specifically interested in these levels, we treat both as categorical variables in modeling. For Fr in particular, 0.3 represents cumulonimbus clouds and 0.052 represents cumulus clouds. See 2.4 for a separate model set that addresses these limitations.

Below, we plot the relationship between the three predictor variables and each of the four response variables (Figure 1 contains graphs for Moment 1. For plots relating to Moments 2-4, please refer to Figures XX-XX in the Appendix). Note, the curves fit to the points are via local polynomial regression.

In general, these seem to be very strong relationships. We also notice that the interaction between `Fr` and `Re` seems to explain a lot of the variance in the response. That is, the relationship between the third variable `St` and the response depends a lot on the specific interaction between `Fr` and `Re`. We will very likely need to include this interaction in any model we build for these data.

Additionally, we notice that the relationship between `St` and the response may benefit from taking the square root of `St`.

2.2 Fitting Process

We used K-fold cross validation with $K = 5$ to choose the model features, exploring linear regression and then nonlinear extensions into polynomial terms and interactions based on the EDA above. Since we only have 89 training observation, we do this in an effort to reduce the likelihood of overfitting. After selecting the features for each moment's model, we then fit the final models on the full training dataset using standard least-squares.

Below, we perform cross validation of a number of candidate models for each moment. Specifically, for each moment, we train a model to predict the moment with the general formula `~ poly(St, degree)*interaction` where `interaction` is the factor interaction between `Fr` and `Re`. We vary the `degree` parameter from 1 to 3. Additionally, we may choose to take the square root of `St` or take the log of the response.

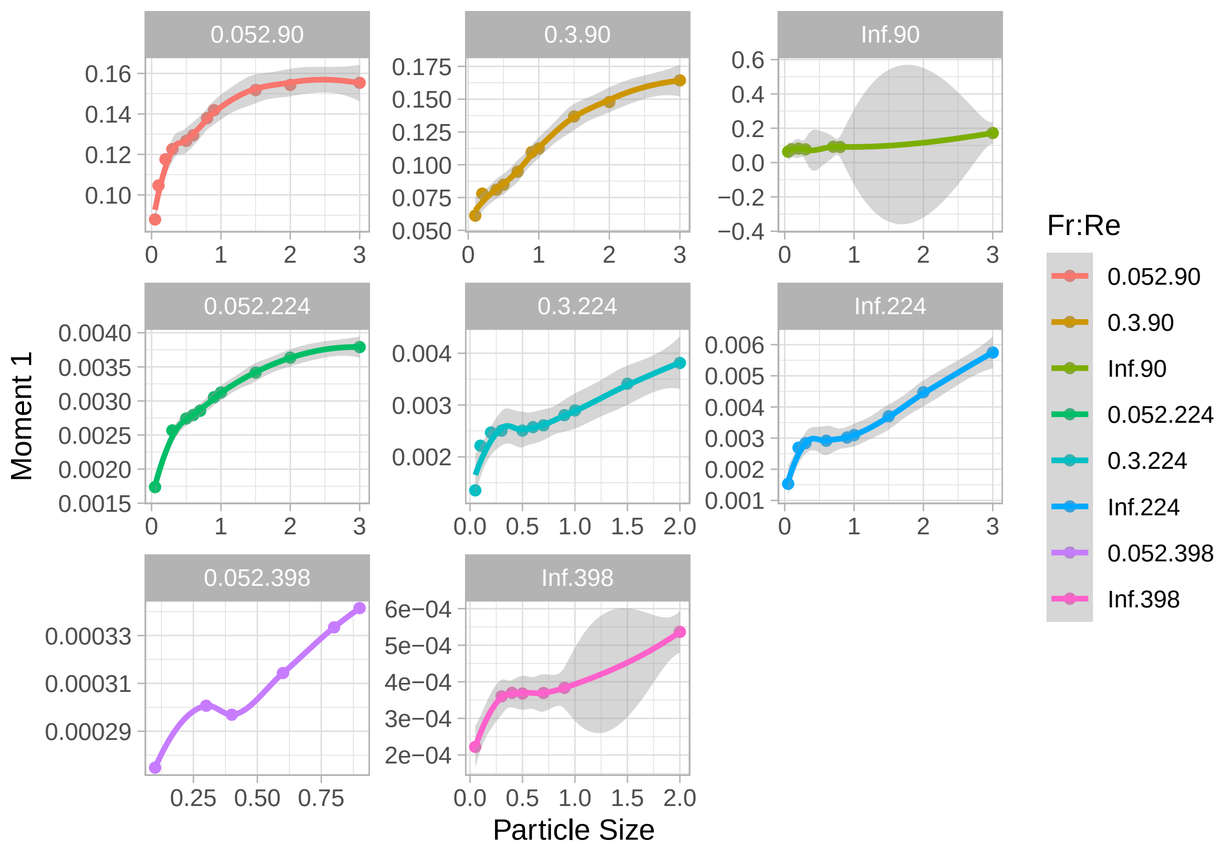
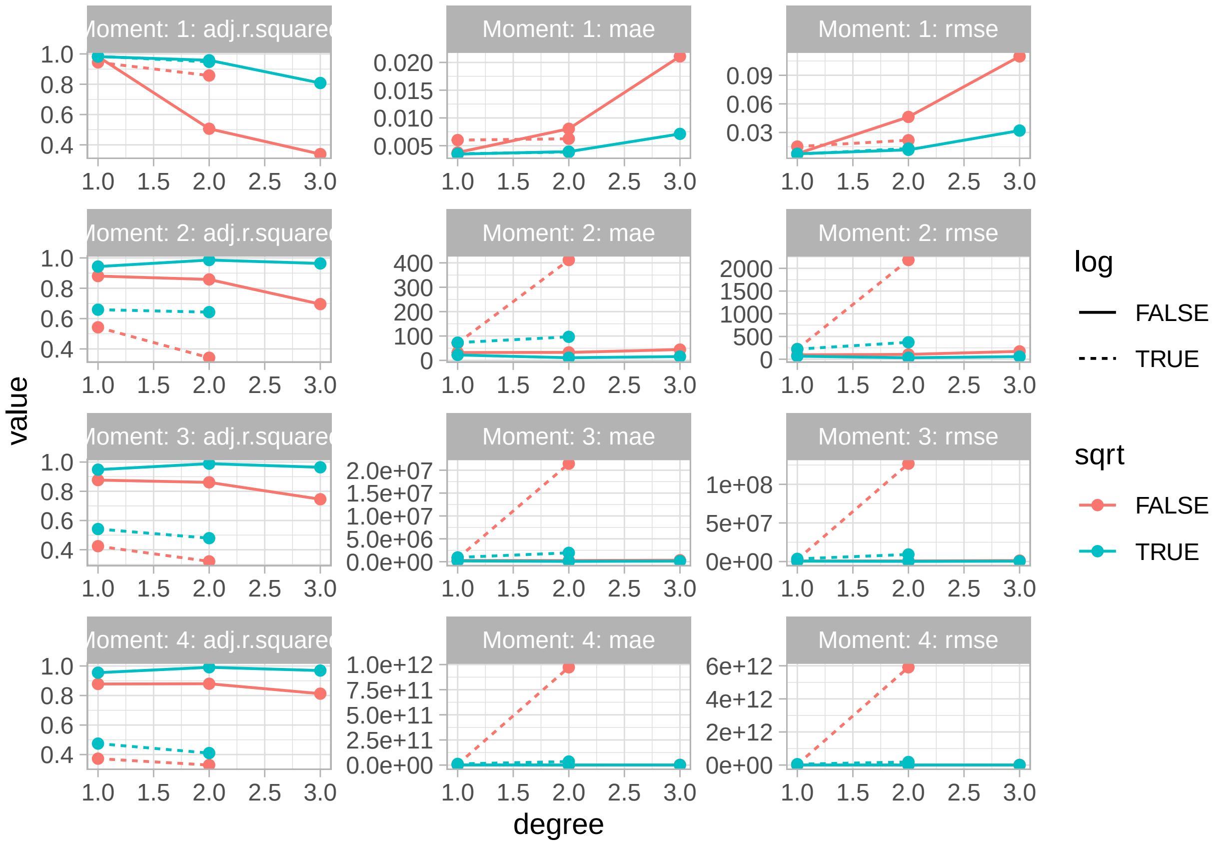


Figure 1: Moment 1 values as a function of particle size at different levels of interaction between Fr and Re.



moment	degree	sqrt	log	name	value
1	1	TRUE	FALSE	mae	0.00348
1	1	TRUE	TRUE	rmse	0.00730
1	1	TRUE	TRUE	adj.r.squared	0.98384
2	2	TRUE	FALSE	rmse	32.42433
2	2	TRUE	FALSE	mae	10.84030
2	2	TRUE	FALSE	adj.r.squared	0.98613
3	2	TRUE	FALSE	rmse	240,845.80324
3	2	TRUE	FALSE	mae	76,364.57174
3	2	TRUE	FALSE	adj.r.squared	0.98910
4	2	TRUE	FALSE	rmse	1,837,866,060.54046
4	2	TRUE	FALSE	mae	558,091,625.13870
4	2	TRUE	FALSE	adj.r.squared	0.99101

2.4 Model Extension

As noted above, extrapolating beyond the three levels of Re and three levels of Fr given may be useful for more general predictions and interpretation, since the actual variables have wide domains (@Jing how to word this). To deal with the limitations of our current models, we also provide the following related models that can be used for extrapolation:

$$R\_moment_1 \sim ns(St, df = 1) * Re * Fr'$$

$$R\_moment_2, R\_moment_3, R\_moment_3 \sim ns(\sqrt{St}, df = 1) * Re * Fr'$$

In these models, Re is numeric and Fr is transformed to a numeric variable on $[0,1]$ using $Fr' = \frac{2}{\pi} * arctan(Fr)$. The form is similar in keeping the significant three-way interaction, except with natural splines to address the poor fits of polynomials at the tails, a location that is especially important in learning about particle behavior in high turbulence. Again, the root and degree are chosen through 5-fold cross validation. See appendix for fitted coefficients.

Results

Model Output:

```
##
## Call:
## lm(formula = central_1 ~ as.factor(Fr) + as.factor(Re) + poly(St,
##     1) * interaction, data = .)
##
## Residuals:
##        Min         1Q     Median         3Q        Max
## -0.0262390 -0.0000713  0.0000154  0.0002443  0.0129019
##
## Coefficients: (4 not defined because of singularities)
##                                    Estimate Std. Error t value Pr(>|t|)
## (Intercept)                        0.095947   0.002907  33.008  < 2e-16 ***
## as.factor(Fr)0.3                   0.005010   0.003425   1.463    0.148
## as.factor(Fr)Inf                   0.000262   0.002217   0.118    0.906
## as.factor(Re)224                  -0.093084   0.002489 -37.394  < 2e-16 ***
## as.factor(Re)398                  -0.095814   0.002748 -34.861  < 2e-16 ***
## poly(St, 1)                        0.004396   0.014016   0.314    0.755
## interaction0.052: 398              0.000195   0.003491   0.056    0.956
## interaction0.052: 90               0.033676   0.003329  10.116 1.55e-15 ***
## interaction0.3: 224               -0.005070   0.003482  -1.456    0.150
## interaction0.3: 90                       NA         NA      NA       NA
## interactionInf: 224                      NA         NA      NA       NA
## interactionInf: 398                      NA         NA      NA       NA
## interactionInf: 90                       NA         NA      NA       NA
## poly(St, 1):interaction0.052: 398 -0.004053   0.020717  -0.196    0.845
## poly(St, 1):interaction0.052: 90   0.136936   0.019962   6.860 1.89e-09 ***
## poly(St, 1):interaction0.3: 224    0.002437   0.025447   0.096    0.924
## poly(St, 1):interaction0.3: 90     0.259529   0.020693  12.542  < 2e-16 ***
## poly(St, 1):interactionInf: 224    0.004275   0.020325   0.210    0.834
## poly(St, 1):interactionInf: 398   -0.003469   0.028921  -0.120    0.905
## poly(St, 1):interactionInf: 90     0.246865   0.021399  11.536  < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.005616 on 73 degrees of freedom
## Multiple R-squared:  0.9916, Adjusted R-squared:  0.9899
## F-statistic: 575.2 on 15 and 73 DF,  p-value: < 2.2e-16
```

```
##
## Call:
## lm(formula = central_2 ~ as.factor(Fr) + as.factor(Re) + poly(St,
##     2) * interaction, data = .)
##
```

```
## Residuals:
##     Min      1Q  Median      3Q     Max
## -63.577  -0.010   0.000   0.011  89.044
##
## Coefficients: (4 not defined because of singularities)
##                                       Estimate Std. Error t value Pr(>|t|)
## (Intercept)                            0.92410    9.92700   0.093    0.926
## as.factor(Fr)0.3                      -0.06581   11.68440  -0.006    0.996
## as.factor(Fr)Inf                      -0.25637    7.49999  -0.034    0.973
## as.factor(Re)224                      -0.61973    8.53408  -0.073    0.942
## as.factor(Re)398                      -0.66125    9.43702  -0.070    0.944
## poly(St, 2)1                           1.02548   47.38085   0.022    0.983
## poly(St, 2)2                          -0.24869   46.96624  -0.005    0.996
## interaction0.052: 398                 -0.25824   11.90579  -0.022    0.983
## interaction0.052: 90                 697.53591   11.35630  61.423   <2e-16 ***
## interaction0.3: 224                   -0.19979   11.91025  -0.017    0.987
## interaction0.3: 90                          NA         NA      NA       NA
## interactionInf: 224                         NA         NA      NA       NA
## interactionInf: 398                         NA         NA      NA       NA
## interactionInf: 90                          NA         NA      NA       NA
## poly(St, 2)1:interaction0.052: 398   -1.01715   81.75775  -0.012    0.990
## poly(St, 2)2:interaction0.052: 398    0.24684   80.93800   0.003    0.998
## poly(St, 2)1:interaction0.052: 90  2603.30410   67.52490  38.553   <2e-16 ***
## poly(St, 2)2:interaction0.052: 90  -792.33489   67.66423 -11.710   <2e-16 ***
## poly(St, 2)1:interaction0.3: 224     -0.89876   79.48124  -0.011    0.991
## poly(St, 2)2:interaction0.3: 224      0.23505   81.79407   0.003    0.998
## poly(St, 2)1:interaction0.3: 90       5.34205   77.87814   0.069    0.946
## poly(St, 2)2:interaction0.3: 90       1.60012   80.14649   0.020    0.984
## poly(St, 2)1:interactionInf: 224     -0.80104   70.45188  -0.011    0.991
## poly(St, 2)2:interactionInf: 224      0.30119   68.45001   0.004    0.997
## poly(St, 2)1:interactionInf: 398     -1.00552   89.82534  -0.011    0.991
## poly(St, 2)2:interactionInf: 398      0.24564   86.54810   0.003    0.998
## poly(St, 2)1:interactionInf: 90       3.66038   72.21510   0.051    0.960
## poly(St, 2)2:interactionInf: 90       2.46518   70.11075   0.035    0.972
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 18.97 on 65 degrees of freedom
## Multiple R-squared:  0.9961, Adjusted R-squared:  0.9947
## F-statistic: 725.9 on 23 and 65 DF,  p-value: < 2.2e-16
```

```
##
## Call:
## lm(formula = central_3 ~ as.factor(Fr) + as.factor(Re) + poly(St,
##     2) * interaction, data = .)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -720016       0       0       0  712324
##
## Coefficients: (4 not defined because of singularities)
##                                       Estimate Std. Error t value Pr(>|t|)
## (Intercept)                          5.206e+01  9.455e+04   0.001        1
## as.factor(Fr)0.3                    -3.853e+01  1.112e+05   0.000        1
```

```
## as.factor(Fr)Inf                    -4.288e+01  7.141e+04  -0.001        1
## as.factor(Re)224                    -8.221e+00  8.129e+04   0.000        1
## as.factor(Re)398                    -9.050e+00  9.021e+04   0.000        1
## poly(St, 2)1                         1.548e+02  4.513e+05   0.000        1
## poly(St, 2)2                        -4.104e+01  4.471e+05   0.000        1
## interaction0.052: 398               -4.293e+01  1.135e+05   0.000        1
## interaction0.052: 90                 5.693e+06  1.081e+05  52.644  < 2e-16 ***
## interaction0.3: 224                 -4.584e+00  1.137e+05   0.000        1
## interaction0.3: 90                          NA         NA      NA       NA
## interactionInf: 224                         NA         NA      NA       NA
## interactionInf: 398                         NA         NA      NA       NA
## interactionInf: 90                          NA         NA      NA       NA
## poly(St, 2)1:interaction0.052: 398 -1.547e+02  7.589e+05   0.000        1
## poly(St, 2)2:interaction0.052: 398  4.097e+01  7.604e+05   0.000        1
## poly(St, 2)1:interaction0.052: 90   2.360e+07  6.432e+05  36.691  < 2e-16 ***
## poly(St, 2)2:interaction0.052: 90  -6.676e+06  6.442e+05 -10.364 2.11e-15 ***
## poly(St, 2)1:interaction0.3: 224   -1.524e+02  7.840e+05   0.000        1
## poly(St, 2)2:interaction0.3: 224    4.081e+01  7.997e+05   0.000        1
## poly(St, 2)1:interaction0.3: 90    -3.317e+01  7.255e+05   0.000        1
## poly(St, 2)2:interaction0.3: 90     7.009e+01  7.462e+05   0.000        1
## poly(St, 2)1:interactionInf: 224   -1.499e+02  6.696e+05   0.000        1
## poly(St, 2)2:interactionInf: 224    4.272e+01  6.536e+05   0.000        1
## poly(St, 2)1:interactionInf: 398   -1.544e+02  8.783e+05   0.000        1
## poly(St, 2)2:interactionInf: 398    4.094e+01  8.513e+05   0.000        1
## poly(St, 2)1:interactionInf: 90    -6.899e+01  6.890e+05   0.000        1
## poly(St, 2)2:interactionInf: 90     8.596e+01  6.617e+05   0.000        1
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 180600 on 65 degrees of freedom
## Multiple R-squared:  0.9949, Adjusted R-squared:  0.9932
## F-statistic: 556.1 on 23 and 65 DF,  p-value: < 2.2e-16
```

```
##
## Call:
## lm(formula = central_4 ~ as.factor(Fr) + as.factor(Re) + poly(St,
##     2) * interaction, data = .)
##
## Residuals:
##        Min         1Q     Median         3Q        Max
## -6.532e+09 -1.000e+01  0.000e+00  5.000e+00  7.352e+09
##
## Coefficients: (4 not defined because of singularities)
##                                       Estimate Std. Error t value Pr(>|t|)
## (Intercept)                          6.451e+03  8.639e+08    0.00        1
## as.factor(Fr)0.3                    -6.217e+03  1.016e+09    0.00        1
## as.factor(Fr)Inf                    -6.310e+03  6.519e+08    0.00        1
## as.factor(Re)224                    -1.215e+02  7.431e+08    0.00        1
## as.factor(Re)398                    -1.382e+02  8.310e+08    0.00        1
## poly(St, 2)1                         2.282e+04  4.121e+09    0.00        1
## poly(St, 2)2                        -7.315e+03  4.083e+09    0.00        1
## interaction0.052: 398               -6.311e+03  1.040e+09    0.00        1
## interaction0.052: 90                 4.667e+10  9.878e+08   47.25   <2e-16 ***
## interaction0.3: 224                 -9.874e+01  1.044e+09    0.00        1
```

```
## interactionInf0.3: 90                          NA         NA      NA       NA
```

```
## interaction0.3: 90                          NA         NA      NA       NA
## interactionInf: 224                         NA         NA      NA       NA
## interactionInf: 398                         NA         NA      NA       NA
## interactionInf: 90                          NA         NA      NA       NA
## poly(St, 2)1:interaction0.052: 398 -2.281e+04  6.643e+09    0.00        1
## poly(St, 2)2:interaction0.052: 398  7.313e+03  6.791e+09    0.00        1
## poly(St, 2)1:interaction0.052: 90   2.081e+11  5.873e+09   35.44   <2e-16 ***
## poly(St, 2)2:interaction0.052: 90  -6.673e+10  5.891e+09  -11.33   <2e-16 ***
## poly(St, 2)1:interaction0.3: 224   -2.277e+04  7.806e+09    0.00        1
## poly(St, 2)2:interaction0.3: 224    7.311e+03  7.756e+09    0.00        1
## poly(St, 2)1:interaction0.3: 90    -2.040e+04  6.415e+09    0.00        1
## poly(St, 2)2:interaction0.3: 90     7.753e+03  6.574e+09    0.00        1
## poly(St, 2)1:interactionInf: 224   -2.270e+04  6.086e+09    0.00        1
## poly(St, 2)2:interactionInf: 224    7.361e+03  5.991e+09    0.00        1
## poly(St, 2)1:interactionInf: 398   -2.281e+04  8.563e+09    0.00        1
## poly(St, 2)2:interactionInf: 398    7.312e+03  8.377e+09    0.00        1
## poly(St, 2)1:interactionInf: 90    -2.119e+04  6.312e+09    0.00        1
## poly(St, 2)2:interactionInf: 90     8.131e+03  5.983e+09    0.00        1
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 1.648e+09 on 65 degrees of freedom
## Multiple R-squared:  0.994,  Adjusted R-squared:  0.9919
## F-statistic: 467.7 on 23 and 65 DF,  p-value: < 2.2e-16
```

Discussion

References

- J. M. J. den Toonder, & Nieuwstadt, F. T. M. (1997, November 1). Reynolds number effects in a turbulent pipe flow for low to moderate re. AIP Publishing. Retrieved October 12, 2021, from https://aip.scitation.org/doi/pdf/10.1063/1.869451.
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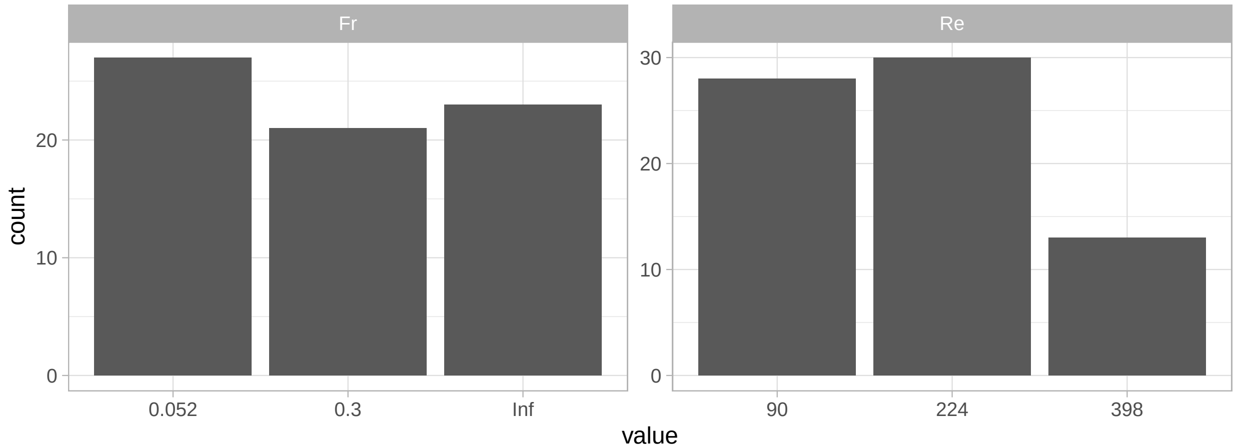
- slides: https://sakai.duke.edu/access/content/group/e1e1b166-17bd-4efc-bdfb-f3909d696910/Case%20Study/Data_Expedition_F2020_Reza_Jon.pdf

Appendix



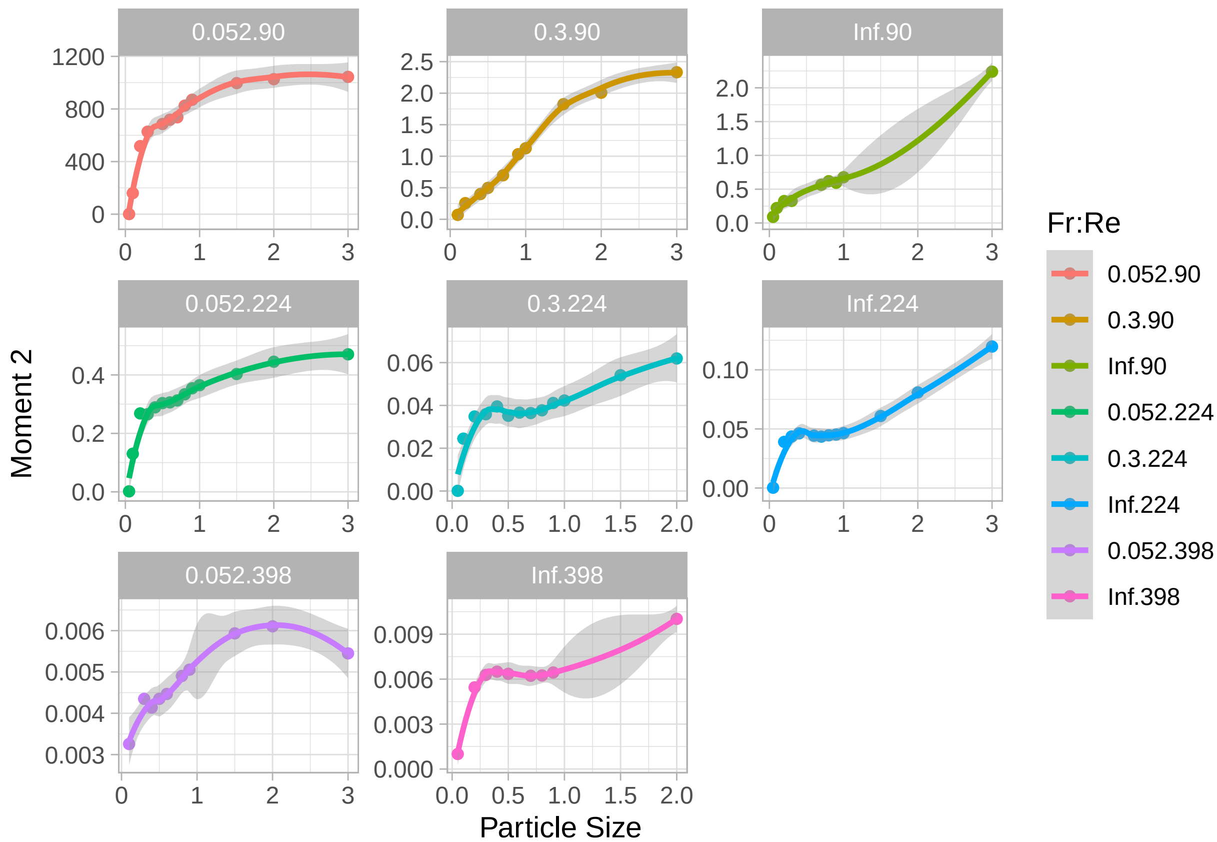


Figure 2: Moment 2 values as a function of particle size at different levels of interaction between Fr and Re.

```
##
## Call:
## lm(formula = R_moment_1 ~ ns(St, df = 1) * Re.numeric * Fr.numeric,
##     data = .)
```

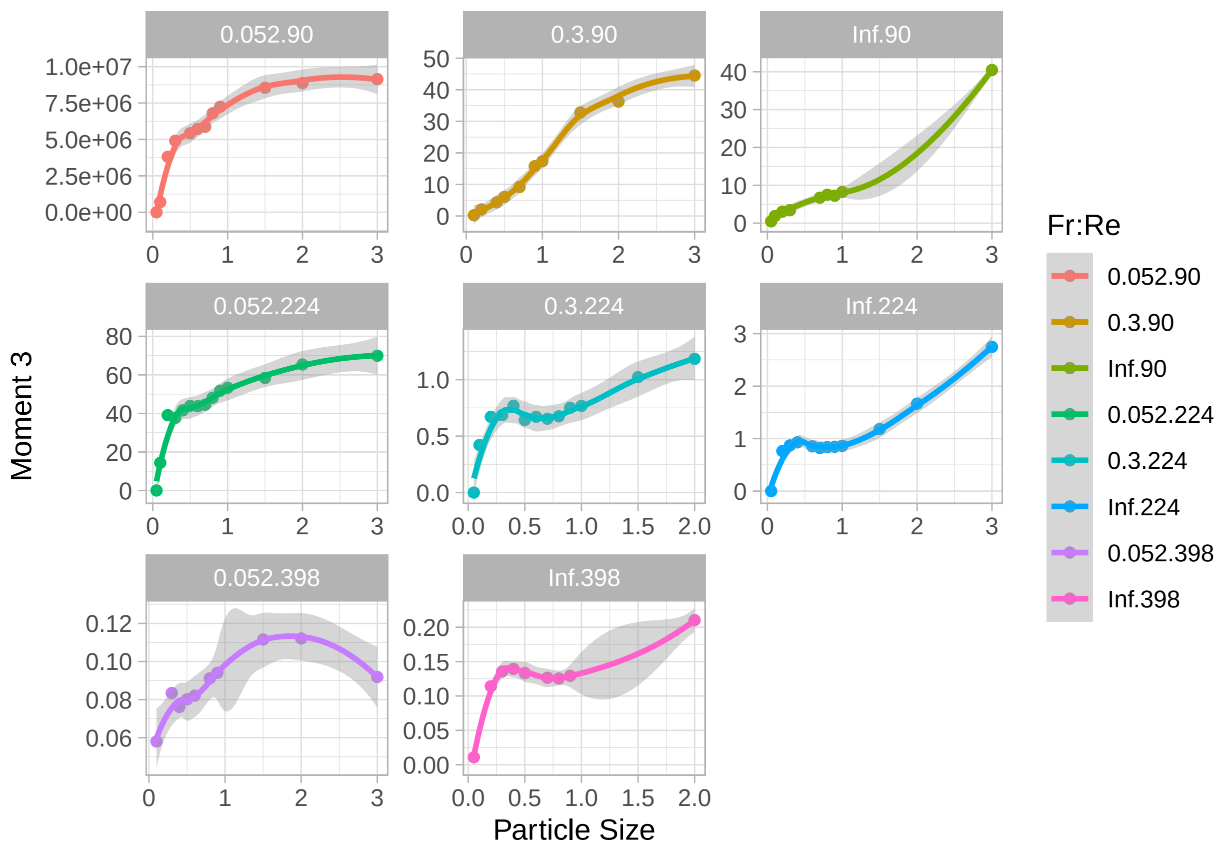


Figure 3: Moment 3 values as a function of particle size at different levels of interaction between Fr and Re.

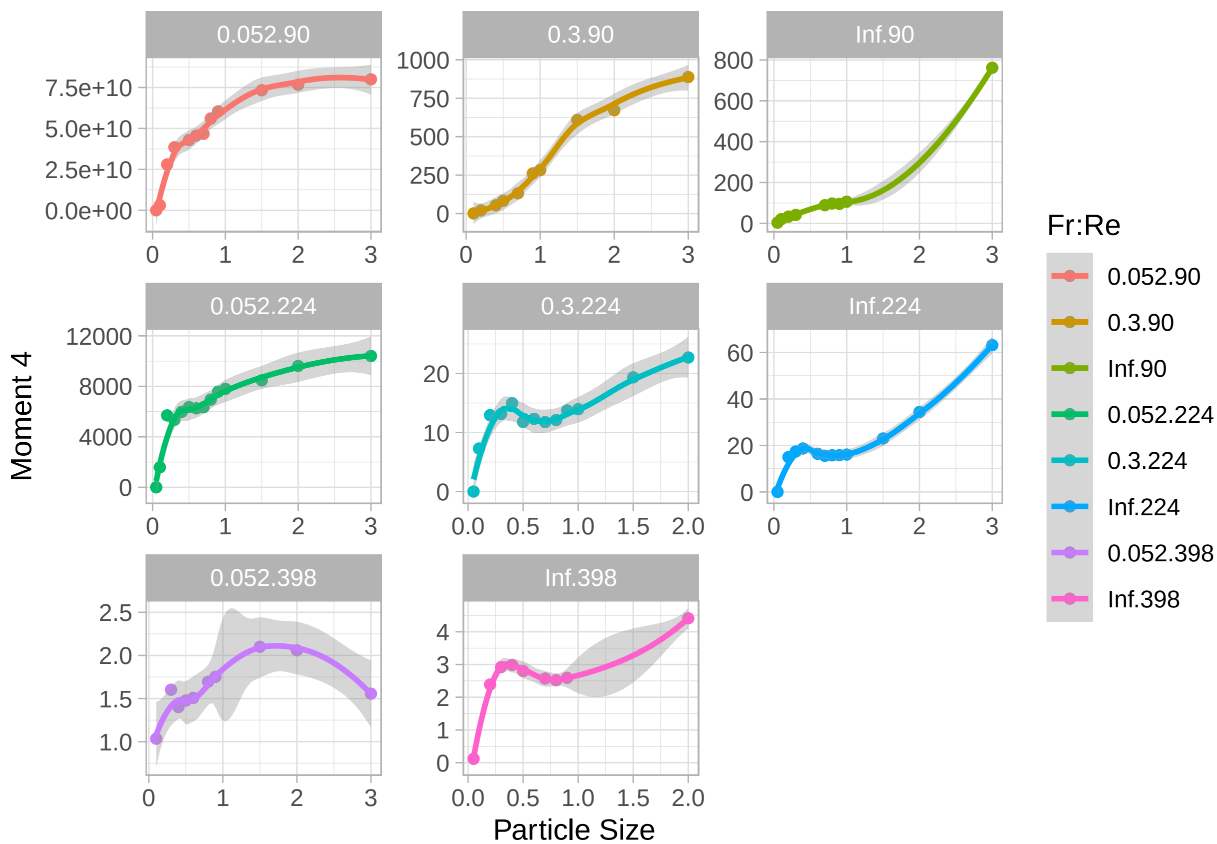


Figure 4: Moment 4 values as a function of particle size at different levels of interaction between Fr and Re.

```
##
## Residuals:
##       Min        1Q    Median        3Q       Max
## -0.065019 -0.028210  0.005928  0.027642  0.051737
##
## Coefficients:
##                                        Estimate Std. Error t value Pr(>|t|)
## (Intercept)                           1.126e-01  1.450e-02   7.764 2.19e-11 ***
## ns(St, df = 1)                        1.096e-01  4.342e-02   2.525   0.0135 *
## Re.numeric                           -3.823e-04  6.211e-05  -6.155 2.72e-08 ***
## Fr.numeric                           -4.745e-02  2.396e-02  -1.980   0.0511 .
## ns(St, df = 1):Re.numeric            -2.513e-04  1.814e-04  -1.385   0.1699
## ns(St, df = 1):Fr.numeric             5.174e-02  7.948e-02   0.651   0.5169
## Re.numeric:Fr.numeric                 2.070e-04  9.559e-05   2.165   0.0333 *
## ns(St, df = 1):Re.numeric:Fr.numeric -3.748e-04  3.397e-04  -1.103   0.2732
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.03225 on 81 degrees of freedom
## Multiple R-squared:  0.6929, Adjusted R-squared:  0.6664
## F-statistic: 26.11 on 7 and 81 DF,  p-value: < 2.2e-16
```

```
##
## Call:
## lm(formula = R_moment_3 ~ ns(St, df = 1) * Re.numeric * Fr.numeric,
##     data = .)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -4261151 -1013391   -17650   469763  4738201
##
## Coefficients:
##                                      Estimate Std. Error t value Pr(>|t|)
## (Intercept)                           1579395    1002500   1.575  0.11905
## ns(St, df = 1)                        7342110    2429982   3.021  0.00337 **
## Re.numeric                              -5849       4369  -1.339  0.18439
## Fr.numeric                           -1641884    1629457  -1.008  0.31663
## ns(St, df = 1):Re.numeric              -20807      10392  -2.002  0.04862 *
## ns(St, df = 1):Fr.numeric            -8824714    4287321  -2.058  0.04277 *
## Re.numeric:Fr.numeric                    5809       6613   0.878  0.38231
## ns(St, df = 1):Re.numeric:Fr.numeric    25642      17867   1.435  0.15508
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 1754000 on 81 degrees of freedom
## Multiple R-squared:  0.4056, Adjusted R-squared:  0.3543
## F-statistic: 7.897 on 7 and 81 DF,  p-value: 2.825e-07
```

```
##
## Call:
## lm(formula = R_moment_4 ~ ns(St, df = 1) * Re.numeric * Fr.numeric,
##     data = .)
##
## Residuals:
```

```
##        Min         1Q     Median         3Q        Max 
## -3.696e+10 -7.454e+09 -1.524e+08  3.926e+09  4.098e+10 
## 
## Coefficients:
##                                       Estimate Std. Error t value Pr(>|t|)   
## (Intercept)                          1.046e+10  8.367e+09   1.250  0.21494   
## ns(St, df = 1)                       6.774e+10  2.028e+10   3.340  0.00127 **
## Re.numeric                          -3.992e+07  3.646e+07  -1.095  0.27687   
## Fr.numeric                          -1.074e+10  1.360e+10  -0.789  0.43218   
## ns(St, df = 1):Re.numeric           -1.943e+08  8.673e+07  -2.241  0.02779 * 
## ns(St, df = 1):Fr.numeric           -8.077e+10  3.578e+10  -2.257  0.02668 * 
## Re.numeric:Fr.numeric                3.895e+07  5.519e+07   0.706  0.48242   
## ns(St, df = 1):Re.numeric:Fr.numeric  2.365e+08  1.491e+08   1.586  0.11658   
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
## 
## Residual standard error: 1.464e+10 on 81 degrees of freedom
## Multiple R-squared:  0.4097, Adjusted R-squared:  0.3587 
## F-statistic: 8.031 on 7 and 81 DF,  p-value: 2.19e-07
```