Case Report

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2021-10-13

1 Introduction

Turbulence is a fundamental concept in fluid mechanics. Irregular, unpredictable, and energy-dissipating, turbulent flow enhances mixing, which leads to non-uniform distribution of particles and cluster formation. Understanding and predicting turbulence has great practical significance in many scientific areas including aeronautical engineering and environmental science.

Existing research suggests that the clustering of particles subject toturbulent flow is mainly determined by three main parameters: Reynolds (Re) number, Froude (Fr) number and Stokes (St) number, which correspond to the intentsity of turbulence, impact of gravitational acceleration, and particle properties.

Despite the importance of turbulence, current understanding of *how* Re, Fr, and St contribute to clustering remains rudimentary. Similation methods like the Direct Numerical Simulation (DNS) of Navier-Stokes equations have been applied, but progress is limited by the time-consuming and computationally-expensive nature of such methodologies (Moin & Mahesh, 1998). Leveraging on generated data, the present study *aims* to build a statistical model that investigates how Re, Fr and St influence particle cluster volume distribution. We hope that our model will 1) enhance our understanding of the relative influence of these parameters in turbulent flow, and 2) enable a quick and efficient prediction of a particle cluster volume distribution without the needs for simulation.

2 Methods

2.1 Data

The data ($n = 89$) for the present study comes from Direct Numerical Simulation. Voronoi Tessellation, a technique that examines general features of individual clusters in the underlying turbulence, was applied to generate a distribution of cluster volumes. The original data contains information regarding the generated distributions in the form of the first four raw moments $E(X)$, $E(X^2)$, $E(X^3)$, and $E(X^4)$, as well as Re, Fr, and St values.

For better interpretability, we transformed the 2nd, 3rd, and 4th raw moments into central moments, which describe the variance (how flow varies over time), skewness (indication of symmetric properties of the flow), and kurtosis of the distribution (how particular cluster volumes deviate). In addition, despite their numerical nature, Fr and Re only contains three levels ($Fr \in \{0.052, 0.3, \inf\}$ and $Re \in \{90, 224, 398\}$) in the data. Given such, the variables were converted into factors (See Section 2.4 for an alternative modeling approach that may overcome this limitation).

2.2 Model Building

A closer examination of the data revealed interesting interactive patterns among the independent and dependent variables. Specifically, St appears to assume a strong, non-linear relationship with each of the moments (Figures S1-S4 in the Appendix). These relationships vary between roughly linear to noticeably curved, potentially quadratic or cubic. In addition, such relationships diverge across different moments, and appears highly influenced by the combined levels of Re and Fr. From the curved shape of the relationship between `St` and the responses, we also noticed that we may benefit from taking certain roots of `St` to make that more linear.

Given the paucity of theoretical background in related field to guide model building, we decided to adopt a k-fold validation approach. This approach would allow us to explore different combinations of polynomial patterns and the interactions observed in our EDA and select the best fit model. Specifically, we used K = 5 given the small sample size at hand to avoid overfitting.

To implement the k-fold cross validation, for each moment, we trained candidate models to predict the moment with the general formula $Moment_i \sim poly(St_i^{(1/root)}, degree) * (Fr, Re)$, varying the *degree* parameter from 1 to 3, *root* from 1 to 6, and testing a log transformation of the response. We combined Fr and Re to form a new interaction variable (Fr, Re) with 9 levels representing all combinations of Fr and Re. We tested the model on each fold, and chose the parameters that give lower root mean squared errors (See Figure 1), with preference for less complexity if the error is similar. After selecting the features for each moment's model, we then fit the final models on the full training dataset using standard least-squares for interpretation.

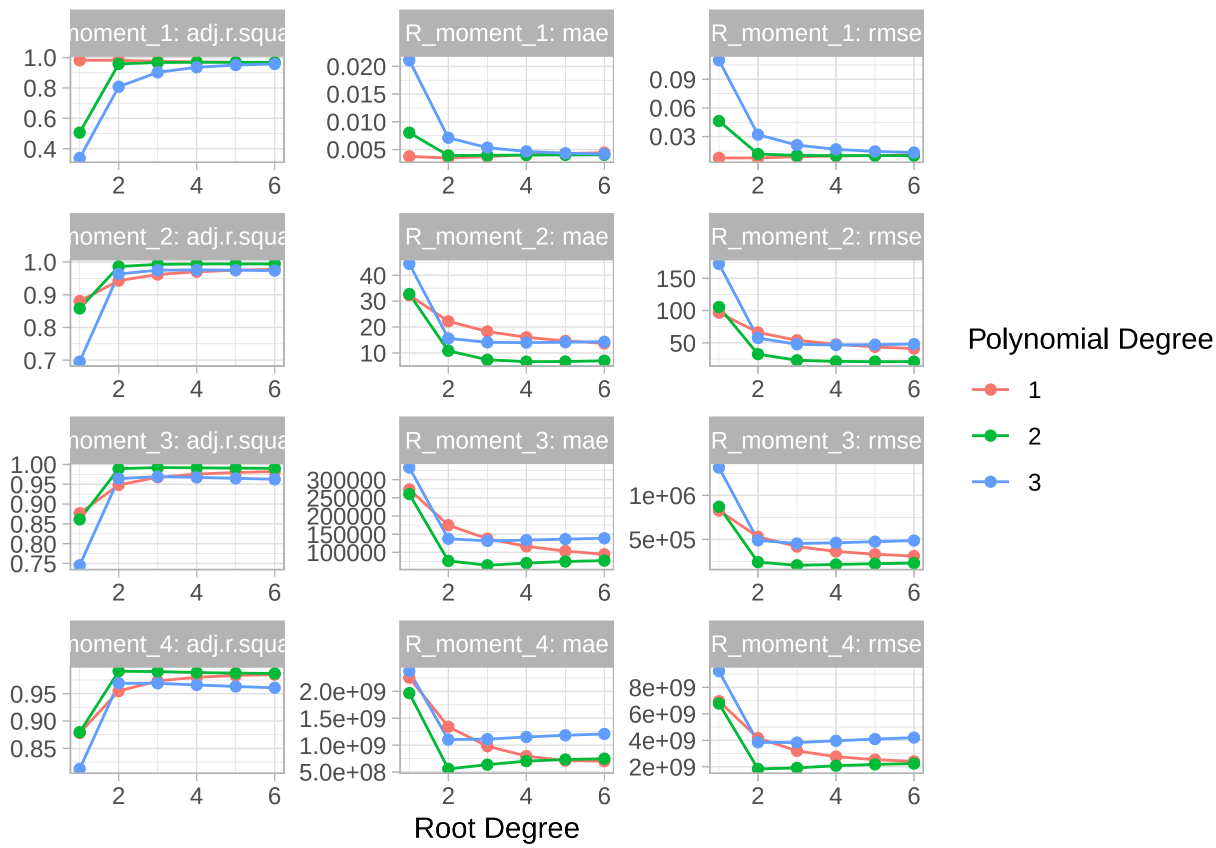

Figure 1. Mean adjusted r-squared value, mean absolute error, and root mean squared error of models for each moment with varying root and polynomial degrees on St. The combination that lead to the lowest root mean squared error was selected as the final model for the moment.

2.3 Final Models

The final models for each moment, based on the k-fold cross-validation approach, are as below:

$$Moment_1 \sim St * (Fr, Re)$$

$$Central\ Moment_2 \sim poly(St^{1/4}, 2) * (Fr, Re)$$
$$Central\ Moment_3 \sim poly(St^{1/3}, 2) * (Fr, Re)$$
$$Central\ Moment_4 \sim poly(\sqrt{St}, 2) * (Fr, Re)$$

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

Selected outputs from the final models of each moment are displayed in Table 1 (See Tables XX-XX for full outputs).

Term	β	SE	t	p value
Moment 1				
interaction0.052: 90	0.127	0.002	57.356	<0.001
interaction0.3: 90	0.098	0.002	41.71	<0.001
interactionInf: 90	0.093	0.002	38.808	<0.001
poly(St, 1):interaction0.052: 90	0.137	0.02	6.86	<0.001
poly(St, 1):interaction0.3: 90	0.26	0.021	12.542	<0.001
poly(St, 1):interactionInf: 90	0.247	0.021	11.536	<0.001
Moment 2				
interaction0.052: 90	698.156	7.492	93.183	<0.001
poly(St, 2)1:interaction0.052: 90	2603.304	67.525	38.553	<0.001
poly(St, 2)2:interaction0.052: 90	-792.335	67.664	-11.71	<0.001
Moment 3				
interaction0.052: 90	5693362.973	71324.394	79.824	<0.001
poly(St, 2)1:interaction0.052: 90	23598512.694	643161.093	36.691	<0.001
poly(St, 2)2:interaction0.052: 90	-6676295.814	644193.322	-10.364	<0.001
Moment 4				
interaction0.052: 90	46674298604.957	650861350.994	71.712	<0.001
poly(St, 2)1:interaction0.052: 90	208144184726.544	5873317691.538	35.439	<0.001

poly(St, 2)2:interaction0.052: 90	-66729237684.868	5891030956.742	-11.327	<0.001

Table 1. Outputs from final models of each moment. Only the significant terms are displayed here given limited space. Please refer to Tables XX-XX in Appendix for full output.

Discussion

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).

However, large Reynolds numbers is highly relevant to real life situations (atmospheric, oceanic turbulence flow).

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). 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).

but it is extremely time consuming and computationally expensive . 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.

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.

For Fr in particular, 0.3 represents cumulonimbus clouds and 0.052 represents cumulus clouds.

References

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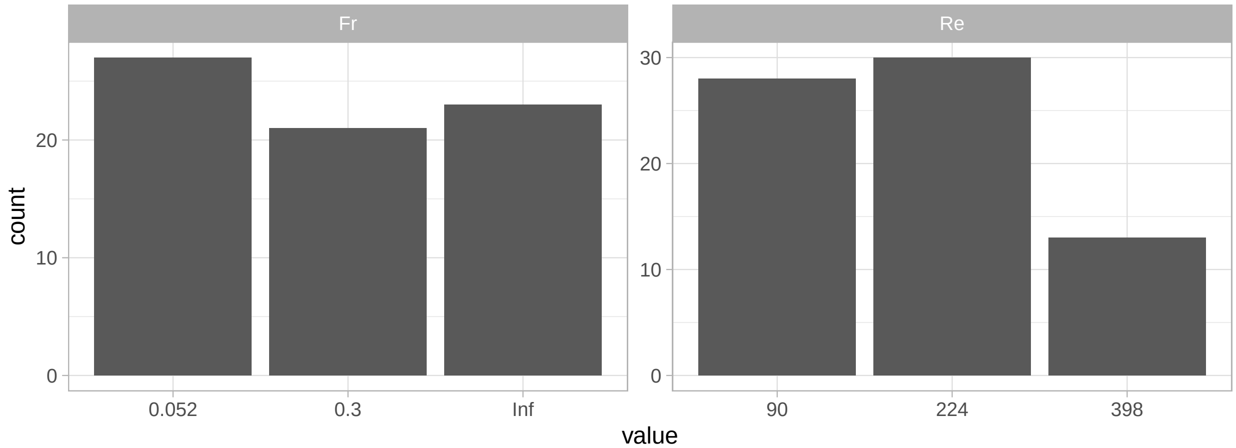
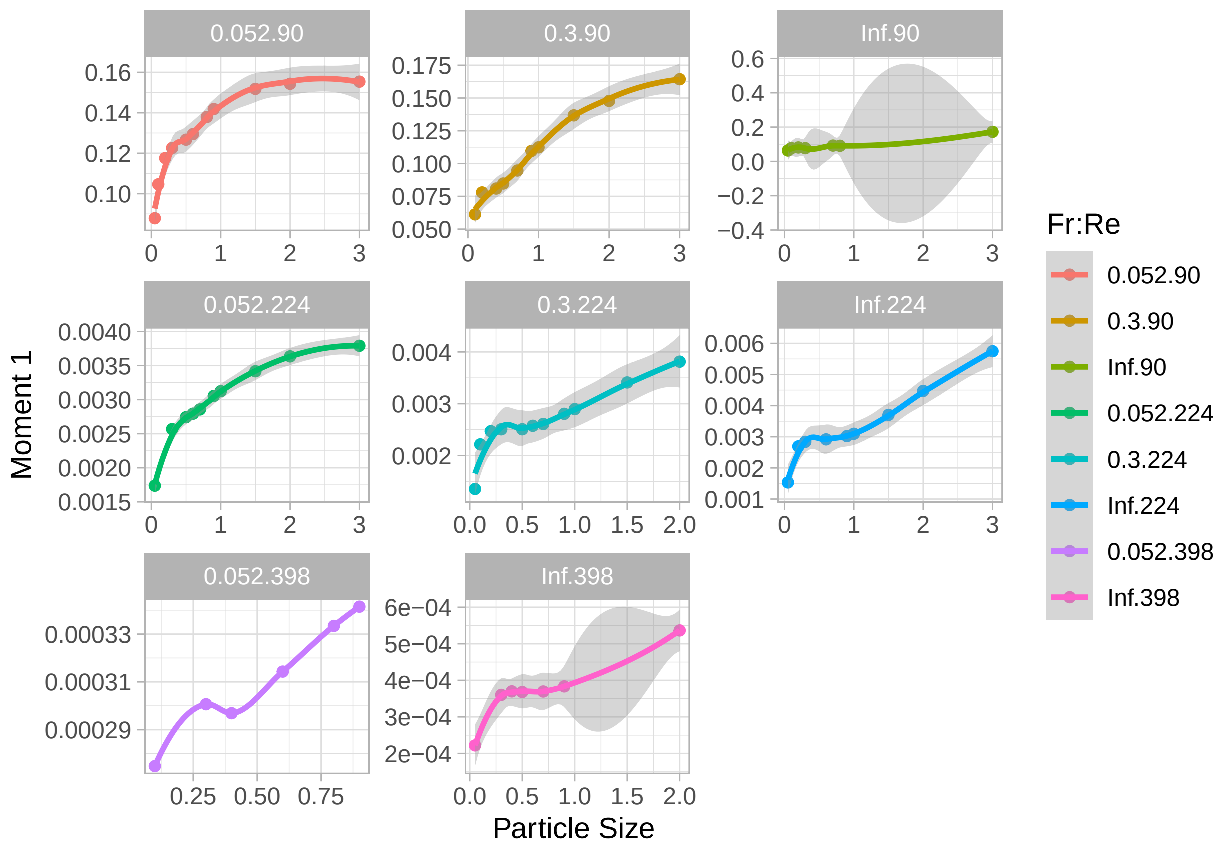
- slides: https://sakai.duke.edu/access/content/group/e1e1b166-17bd-4efc-bdfb-f3909d696910/Case%20Study/Data_Expedition_F2020_Reza_Jon.pdf

Appendix





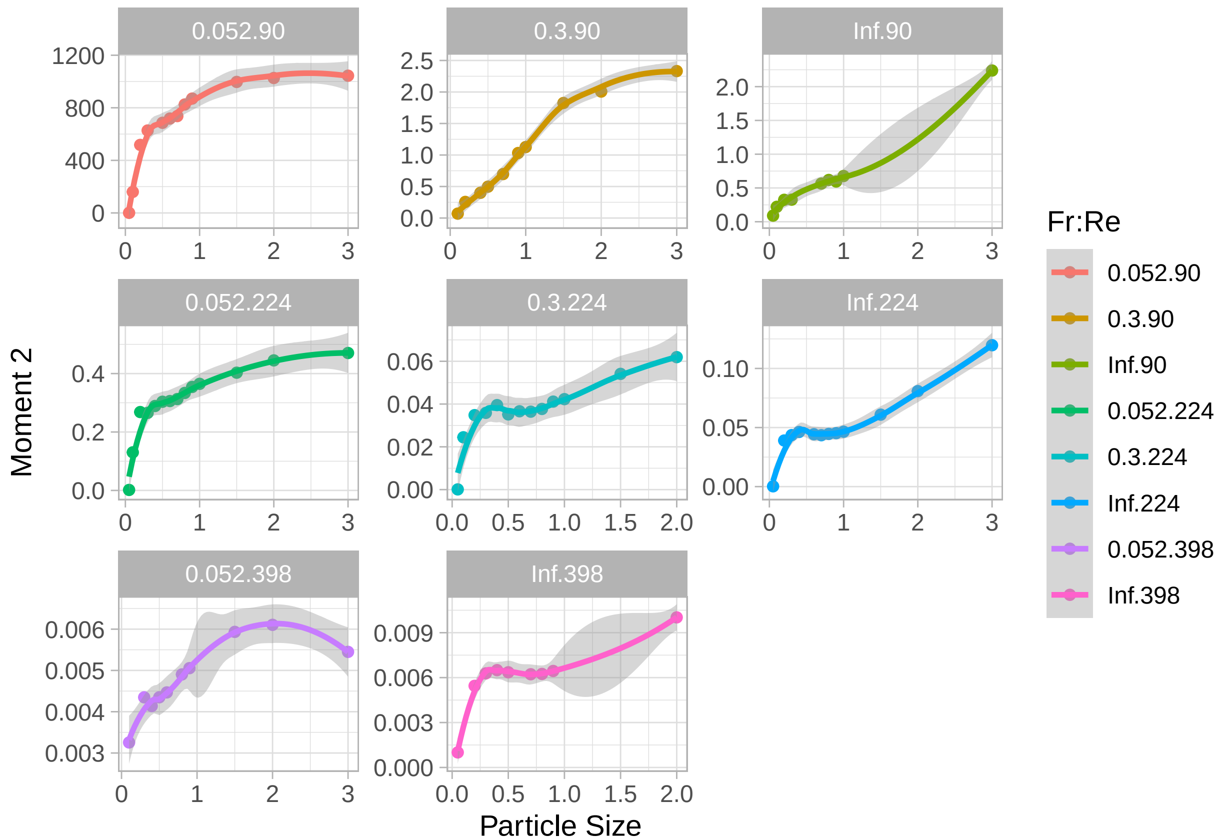
Moment 1 values as a function of particle size at different levels of interaction between Fr and Re.

moment	degree	root	log	name	value
R_moment_1	1	2	FALSE	rmse	0.00764
R_moment_1	1	2	FALSE	mae	0.00348
R_moment_1	1	2	FALSE	adj.r.squared	0.98223
R_moment_2	2	4	FALSE	mae	6.64671

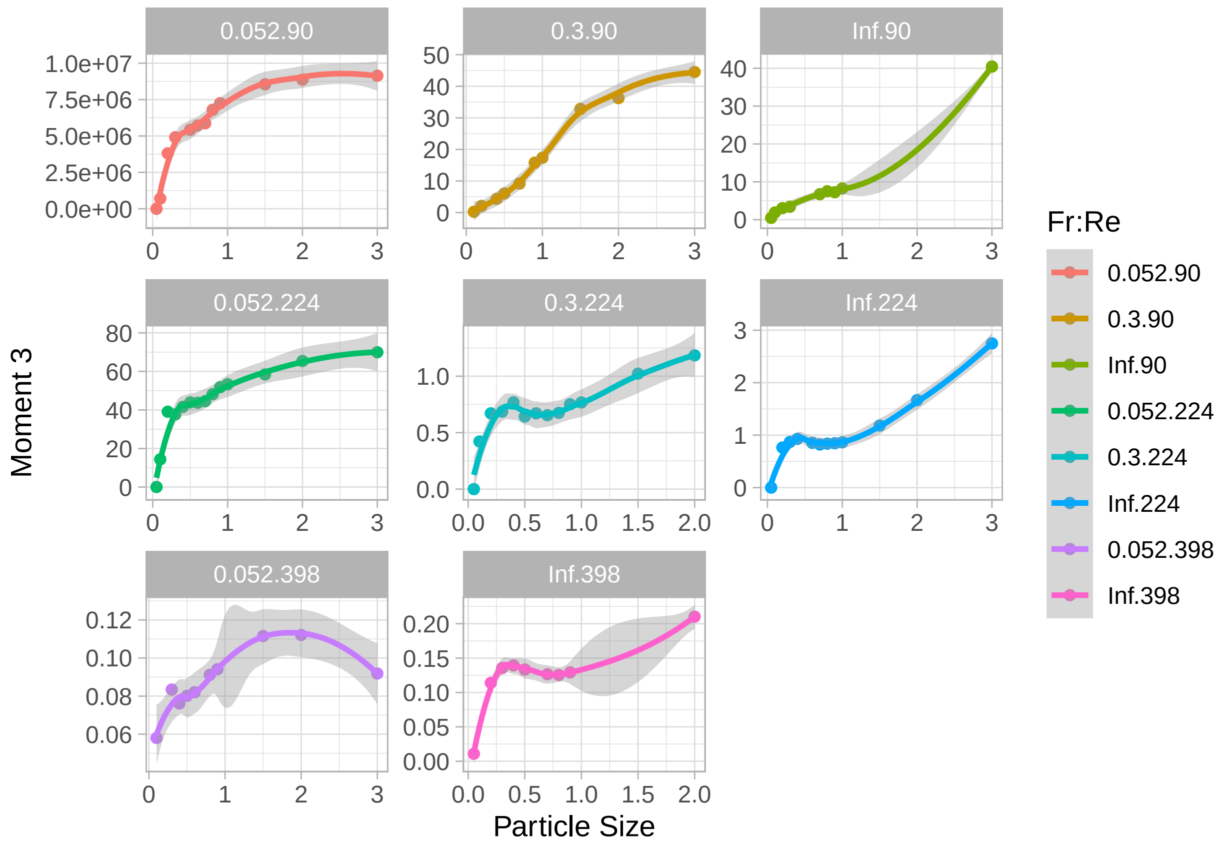
moment	degree	root	log	name	value
R_moment_2	2	5	FALSE	rmse	20.85942
R_moment_2	2	5	FALSE	adj.r.squared	0.99428
R_moment_3	2	3	FALSE	rmse	205,406.99660
R_moment_3	2	3	FALSE	mae	64,341.96016
R_moment_3	2	3	FALSE	adj.r.squared	0.99206
R_moment_4	2	2	FALSE	rmse	1,837,891,935.00114
R_moment_4	2	2	FALSE	mae	558,101,834.24670
R_moment_4	2	2	FALSE	adj.r.squared	0.99101

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

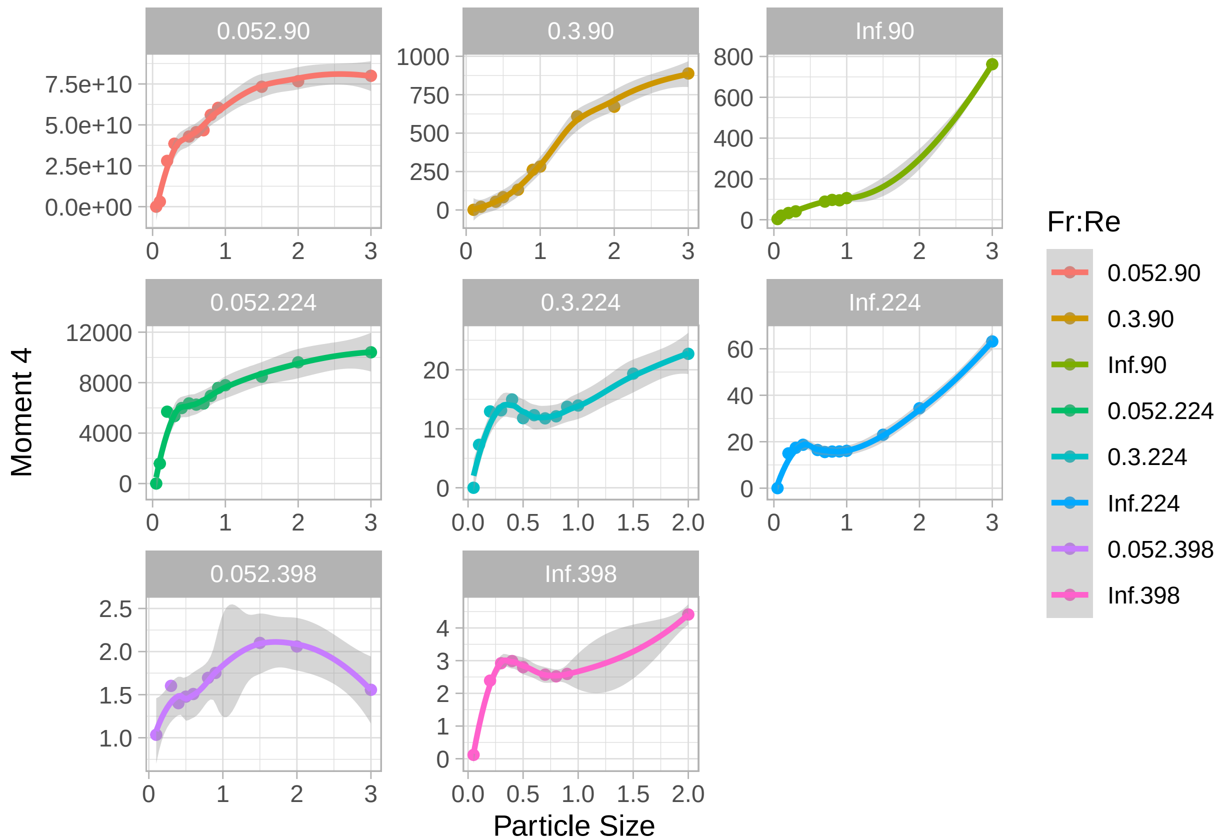
```
##
## Call:
## lm(formula = R_moment_3 ~ ns(St, df = 1) * Re.numeric * Fr.numeric,
##     data = .)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -4261151 -1013391   -17650   469763  4738201
##
## Coefficients:
##                                      Estimate Std. Error t value 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 *
```



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



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



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

```
## 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
```