

ST_518 Project

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Executive Summary

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Introduction

For this paper we have been presented with data gathered on the dissolving cold medicine in water. The dataset contains dissolving characteristics of different cold medicine brands done under various environmental conditions. The goal of this paper is to answer the following questions:

- Are the dissolving characteristics different between brands?
- Does temperature of the water influence dissolving characteristics? If so, is there an interaction effect between brand and temperature?
- Does stirring influence dissolving times and is there an interaction with the other two effects?

Experimental Design

Data used for this study was obtained from an experiment called the ‘Effervescent Experiment’. The experiment was conducted on two different brands of cold medicine, ‘Name’ and ‘Store’. Each brand was dissolved in water at three different but evenly spaced temperatures, 6°C, 23°C, and 40°C. Data was gathered on each combination of brand and temperature using 4 replications. The experiment was then repeated with the introduction of stirring as a blocking factor. Samples were stirred using a magnetic stirrer spinning at 350 rpm. The data was then tabulated and made available for this analysis.

Exploratory Data Analysis

Summary

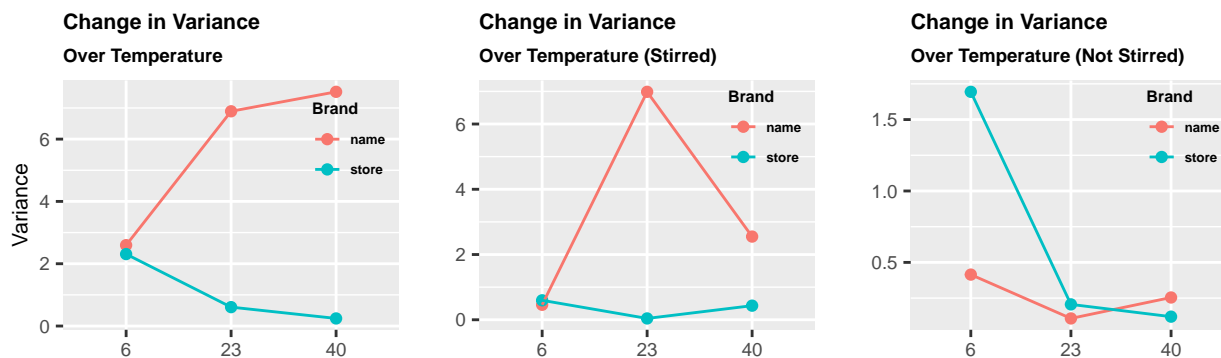
In total, the provided dataset contains 48 rows and 5 columns. The 5 columns include 3 explanatory categorical variables (Brand, Temp in °C, and Stirring), a single continuous response variable (Time, in minutes) and one descriptor (order). Prior to analysis, the data will be explored to gain a better understanding of what to expect and, more importantly, check for any potential violations of analytical assumptions.

From the summary statistics table (see Appendix 1, Table 1), we can see that each group has exactly 4 entries, eliminating concerns with respect to design imbalance. Constructing a means table for the data without taking into account stirring, we can see that there does appear to be a disparity between the mean dissolving times of store brand cold medications when compared to name brand.

Table 1: Means Table

Temp	Name	Store	Temp. Mean
6	77.60	78.41	78.01
23	74.53	66.85	70.69
40	68.20	59.04	63.62
Brand Mean	73.44	68.10	70.77

When inspecting the marginal means of store versus name brand, we find that store brand dissolves in less time, on average, than the name brand. This disparity becomes more pronounced as the effect of temperature is introduced. It was observed that increasing temperature has a more dramatic effect on store brand medicine than name brand. Dissolving time for store brand medicine drops from 78.42 to 59.04 (Δ of -19.38) seconds across a temperature change from 6°C to 40°C. Whereas, name brand medicine only drops from 77.60 to 68.20 (Δ of -9.40 seconds) across the same temperature change.



Next, consider the range in variability at each factor and level. The range in values of the variance is 6.9458; an interesting result considering nine of the twelve observable variances fall within a range of 0.04 and 1.69. The variability between observations of name brand cold medicines are elevated, especially in cases when the observation was stirred at 23°C and 40°C. Variance of non-stirred observations, particularly within temperature values of 23°C and 40°C, are noticeably lower than their stirred counterparts within the same brand. The variance seems to jump by a large amount between the groups.

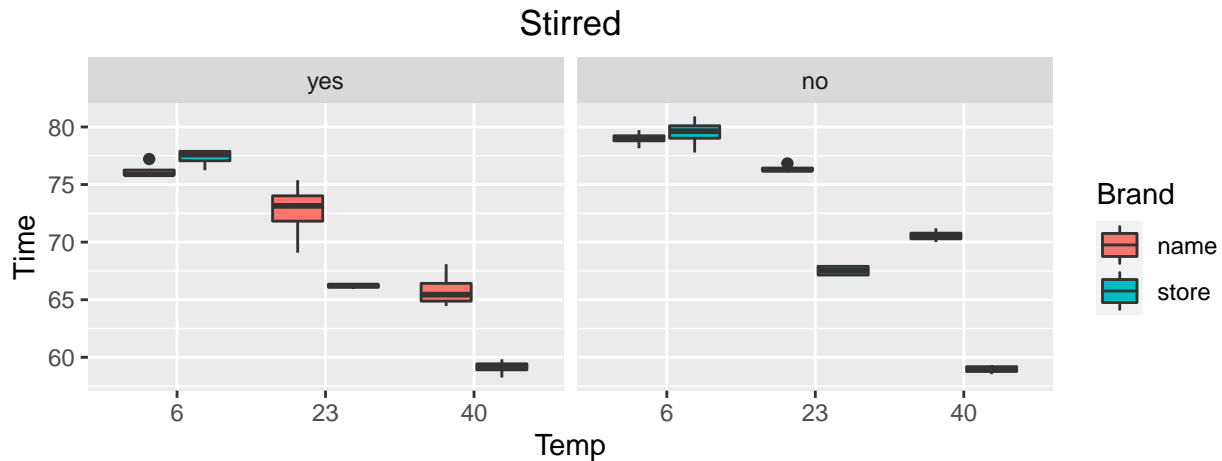
The scatterplots show there is a noticeable increase in the variance of the name brand medicine in the stirred block versus the non stirred especially at higher temperatures. Turning our attention to the boxplot we can observe that stirring produced a decrease in the mean differences of brand within each temperature grouping. Earlier, we had introduced an insight from the summary statistics output indicating an inverse relationship between temperature and dissolve time—as temperature increases dissolve time decreases. The boxplot reinforces this idea.

Further contextualizing central tendency and spread, we can see this illustrated in a different perspective by grouping effects together. Take note that temperature has the smallest set of ranges, both at each level and as a whole when compared to brand type and stirring effect. There is not a lot of variability among temperatures compared to the other effects though they are different enough to identify an irregular increase as temperature increases. The range of values provides additional context to the data's story; data points when focused only on temperature groups tend to be within a smaller range of each other indicating less variability; meanwhile, brand and stirring effects have a wider distribution and more variability—outliers withstanding.

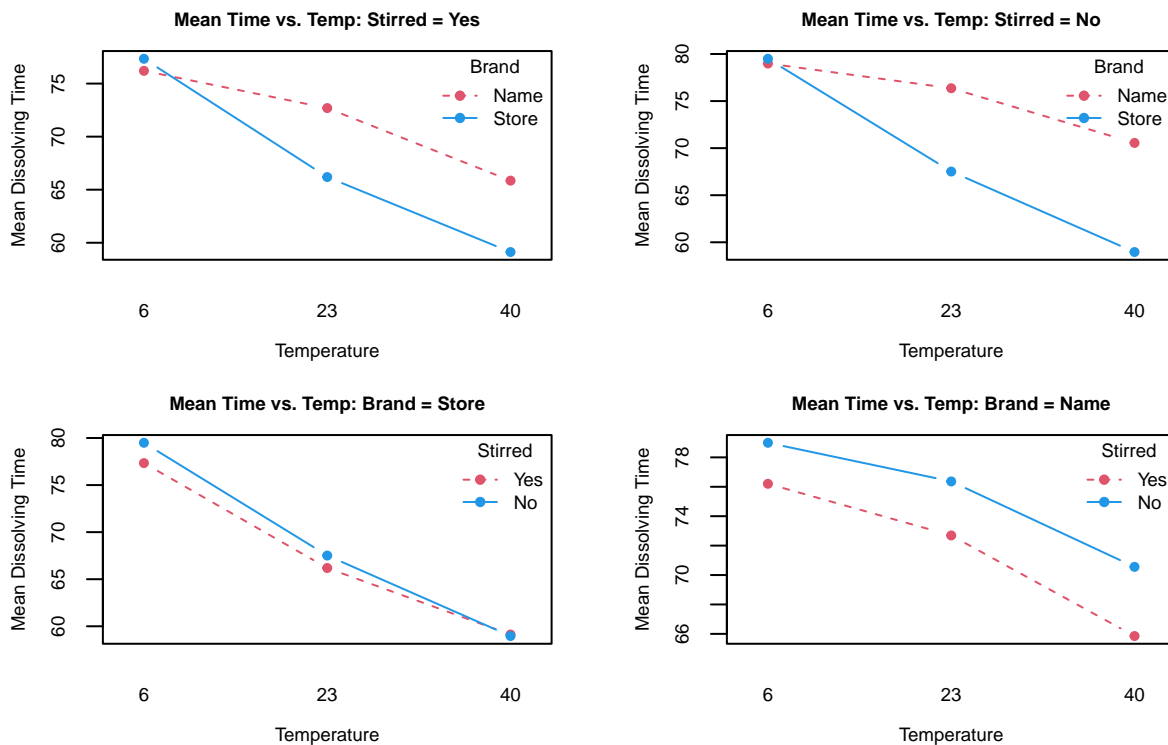
Interactions

From the boxplots below, we can immediately see that stirring seems to increase the variance of the name-brand medicine—while also decreasing the mean differences of brand observations within each temperature grouping. An interaction effect between temperature and brand can be deduced if lines are drawn through the centers of the boxes. Earlier, we had introduced an insight from the summary statistics output indicating an inverse relationship between temperature and dissolve time—as temperature increases dissolve time decreases. The boxplot reinforces this idea. We can also claim that temperature has an inverse effect on dissolving times whether stirring is present or not—indications of temperature having a strong effect on dissolving time by itself. Stirring might have an additive effect regardless of temperature.

It is simply conjectured at this point, however, we noticed that observations of dissolve time while stirring the water seems to have increased the name brand variability, while not stirring the water seems to have increased the store brand variability. Perhaps worth looking into the blocking effects of stirred on variability at various temperatures.

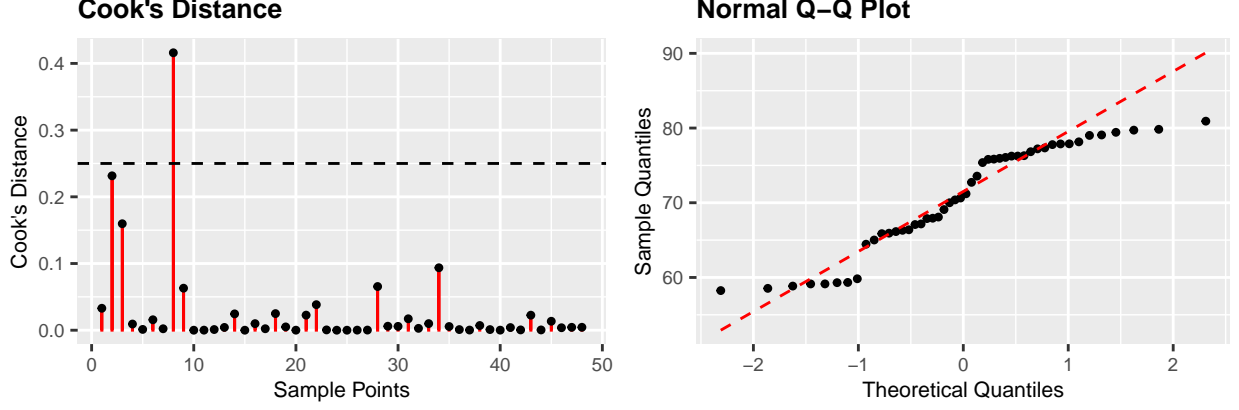


The possible interaction between brand and temperature becomes even more noticeable in the preceding three-factor interaction plots. Specifically, the brand and temperature interaction can be seen when the temperature increases. The slope for the store brand has a more pronounced negative slope than the slope of the name brand. In addition, there might be a slight three-factor interaction between brand, temperature, and stirring as the name and store brand lines appear to be closer together in the stirred=yes plot than the stirred=no plot.



Assumptions and Violations

In reference to the boxplots, we were able to see a small number of outliers. To confirm if there is any concern we plotted the Cook's Distance for each point based on a full linear model. Point 8 has a higher Cook's distance than the rest of the points which may require removal for analysis if it is suspected of causing issues in the analysis. This would have to be weighed against the risks caused by introducing imbalances.



Finally, we check the normality of the data. Here a Q-Q plot is generated for the full model residuals. The data appears to suffer from heavy tails, multimodality and/or gaps in data between the left tail and the center. Since downstream analysis hinges on the assumption that our data is normally distributed, these issues may pose a problem.

Analysis and Results

Model Development

The following models were developed and analyzed for this paper:

$$\text{Model 1: } Y_{ijkl} = \mu + \alpha_i + \beta_j + \gamma_k + (\alpha\beta)_{ij} + (\alpha\gamma)_{ik} + (\gamma\beta)_{jk} + (\alpha\beta\gamma)_{ijk} + \epsilon_{ijkl}$$

$$\text{Model 2: } Y_{ijkl} = \mu + \alpha_i + \beta_j + \gamma_k + (\alpha\beta)_{ij} + \epsilon_{ijkl}$$

$$\text{Model 3: } Y_{ijkl} = \mu + \alpha_i + \beta_j + \gamma_k + \epsilon_{ijkl}$$

Where α is brand effect, β is temperature effect, γ is stir effect. i, j, k are (1, 2), (1,2,3), and (1,2), respectively. ϵ_{ijkl} is assumed to be normally distributed with a μ_ϵ of 0 and a variance of σ_ϵ^2 . μ is the overall mean and is an unknown value.

Mixed Effects models:

$$\text{Model 4: } Y_{ijk} = \mu + \alpha_i + B_j + (\alpha B)_{ij} + \epsilon_{ijk}$$

Where brand is fixed and temperature is random.

$$\text{Model 5: } Y_{ijk} = \mu + A_i + \beta_j + (A\beta)_{ij} + \epsilon_{ijk}$$

Where brand is random and temperature is fixed.

$$\text{Model 6: } Y_{ijk} = \mu + A_i + B_j + (AB)_{ij} + \epsilon_{ijk}$$

Where both brand and temperature are random.

With order as a factor:

$$\text{Model 7: } Y_{ijklm} = \mu + \alpha_i + \beta_j + \gamma_k + \nu_l + (\alpha\beta)_{ij} + \epsilon_{ijklm}$$

Similar to model 2, but with an introduced effect, ν , to represent order.

$$\text{Model 8: } Y_{ijklm} = \mu + \alpha_i + \beta_j + \gamma_k + \nu_l + (\alpha\beta)_{ij} + (\alpha\gamma)_{ik} + (\gamma\beta)_{jk} + (\alpha\beta\gamma)_{ijk} + \epsilon_{ijklm}$$

Similar to model 1, but with an introduced effect, ν , to represent order.

Model Selection

	Root MSE	R^2	adj R^2	AIC	BIC
Model1	1.075	0.982	0.977	155.337	179.663
Model2	1.319	0.970	0.966	171.198	186.168

	Root MSE	R^2	adj R^2	AIC	BIC
Model3	2.655	0.872	0.860	236.681	247.908
Model7	1.303	0.971	0.966	170.872	187.713
Model8	1.087	0.983	0.977	157.056	183.252

The mixed/random effects Models 4, 5, 6 all had Root MSE=1.833 (see Appendix 1, Table 13).

ANOVA Analysis

Table 3: Model 1: ANOVA Table

	Df	Sum Sq	Mean Sq	F value	Pr(>F)
Brand	1	342.007	342.007	296.041	0.000
Temp	2	1654.737	827.368	716.169	0.000
Stirred	1	69.888	69.888	60.495	0.000
Brand:Temp	2	231.852	115.926	100.345	0.000
Brand:Stirred	1	20.510	20.510	17.753	0.000
Temp:Stirred	2	0.125	0.062	0.054	0.948
Brand:Temp:Stirred	2	9.056	4.528	3.919	0.029
Residuals	36	41.590	1.155	NA	NA

Our null and alternative hypotheses are:

H_o : All the means are.....

H_a : Not the null

We found that.....

Contrasts

Conducting a linear contrast analysis on each of the explanatory variables reveals that there are significant differences between groups based on factors, see Appendix 1 Table 2, 3, 4, and 5 for full results.

In the first case, we contrasted the means of stirred versus not stirred. Here the difference in means is -2.41 with an upper 95% confidence limit of -3.04 and a lower 95% CI limit of -1.78. In other words, on average stirring medicine reduces dissolving time by between 3.04 and 1.78 minutes regardless of brand or temperature. When looking only at brand, name brand dissolving times were on average between 4.71 and 5.97 (95% CI) minutes slower than store brand. Since neither of the intervals contained zero we can conclude that there is a difference between brands and between the presence of stirring.

While significant for both store and name brands, stirring had more of an impact to dissolving times for name brand than it did for the store brand. Stirring reduced name brand dissolving times by 2.83 and 4.61 minutes whereas for the store brand that interval was 0.22 and 2 minutes.

A similar analysis was completed for the three levels of temperature. Completing a contrast analysis using a Bonferroni correction we found that in pairwise cases each level was significantly different from the other. The 95% confidence limits were (6.25, 8.38), (13.32, 15.44), and (6.00, 8.13) for the pair wise comparisons of $6^\circ C$ vs $23^\circ C$, $6^\circ C$ vs $40^\circ C$, and $23^\circ C$ vs $40^\circ C$, respectively. Zero did not fall in any of those ranges. When comparing individual levels versus the remainder of the group, $23^\circ C$ was found not to be significantly different from the rest of the levels. That confidence interval ranged from -1.04 to 0.80 minutes of dissolving time. Due to that, we do not have enough evidence to say $23^\circ C$ is different from either $6^\circ C$ or $40^\circ C$.

Random Effects Analysis

Expanding Table 20 from Appendix 1 to include portion of variance due to effect, the following table is produced:

Cov Parm	Estimate	Portion
Brand	9.420	0.132
Temp	44.465	0.623
Brand*Temp	14.071	0.197
Residual	3.361	0.047

The results from the ANOVA analysis are based on the following:

For brand:

$H_o : \sigma_\alpha^2$ is equal to zero

$H_a : \sigma_\alpha^2$ is not equal to zero

For temperature:

$H_o : \sigma_\beta^2$ is equal to zero

$H_a : \sigma_\beta^2$ is not equal to zero

For interaction:

$H_o : \sigma_{\alpha\beta}^2$ is equal to zero

$H_a : \sigma_{\alpha\beta}^2$ is not equal to zero

The calculated critical f score is 19 using an α of 0.05 and (2, 2) degrees of freedom. The f score for brand and for temperature were below the critical f score. Brand produced an f score of 2.95 and Temperature produced a score of 7.14. In both cases, the null hypothesis was not rejected, therefore, $\sigma_\alpha^2 = \sigma_\beta^2 = 0$. On the other hand, the critical value for the interaction variance is 3.2199423 using an α of 0.05 and (2, 42) degrees of freedom. At a value of 34.5, we are able to reject the null hypothesis in favor of the alternative. The variance associated with the interaction effect is significant.

Further analysis determines, temperature is responsible for the largest portion of total variance. σ_β^2 , at value of 44.465, explains 62.3% of the total variance ($\hat{\sigma}_{total}^2$ being 71.32).

The overall dissolving meantime, $\hat{Y}_{...}$, was found to be 70.773. The standard error of that value, $SE(\mu)$ was calculated to be 4.684748. From that we find the 95% confidence limit is ± 3.705803 .

\widehat{CV} was found to be 0.119.

Conclusion

Are we able to answer the questions in the introduction?

Appendix I: Analysis Tables and Figures

Table 5: Data Summary Table

Brand	Temp	Stirred	Min	25%	Mean	Median	75%	Max	Range	Var	n
name	6	yes	75.80973	75.83358	76.20241	75.89223	76.26107	77.21547	1.4057377	0.4593492	4
name	6	no	78.15246	78.79910	78.99061	79.04435	79.23586	79.72130	1.5688327	0.4146440	4
name	23	yes	69.08937	71.82180	72.69145	73.14894	74.01859	75.37855	6.2891789	6.9869087	4
name	23	no	76.06895	76.20492	76.36351	76.27622	76.43481	76.83265	0.7636940	0.1078134	4
name	40	yes	64.45156	64.87321	65.85343	65.43863	66.41886	68.08492	3.6333543	2.5499751	4
name	40	no	69.99943	70.28754	70.55511	70.50947	70.77705	71.20207	1.2026434	0.2544033	4
store	6	yes	76.24402	77.06561	77.33703	77.60659	77.87801	77.89089	1.6468708	0.5964884	4
store	6	no	77.78345	79.01994	79.49240	79.63219	80.10465	80.92176	3.1383169	1.6942517	4
store	23	yes	65.92809	66.08831	66.19126	66.22629	66.32923	66.38436	0.4562787	0.0411024	4
store	23	no	67.08353	67.14393	67.51552	67.52360	67.89520	67.93138	0.8478521	0.2060739	4
store	40	yes	58.24407	58.90895	59.12529	59.21659	59.43293	59.82388	1.5798100	0.4320148	4
store	40	no	58.53920	58.76884	58.96347	58.99050	59.18513	59.33370	0.7945066	0.1202191	4

Brand	Mean	Var	Max	Min	Spread
name	73.44276	21.13144	79.72130	64.45156	15.26973
store	68.10416	67.03190	80.92176	58.24407	22.67769

Temp	Mean	Var	Max	Min	Spread
6	78.00561	2.467426	80.92176	75.80973	5.112037
23	70.69044	19.204515	76.83265	65.92809	10.904559
40	63.62433	25.996561	71.20207	58.24407	12.958001

Brand	Temp	Mean	Var	Max	Min	Spread
name	6	77.59651	2.5957290	79.72130	75.80973	3.911567
name	23	74.52748	6.8931729	76.83265	69.08937	7.743272
name	40	68.20427	7.5178162	71.20207	64.45156	6.750513
store	6	78.41471	2.3090692	80.92176	76.24402	4.677741
store	23	66.85339	0.6069845	67.93138	65.92809	2.003292
store	40	59.04438	0.2441527	59.82388	58.24407	1.579810

Brand	Stirred	Mean	Var	Max	Min	Spread
name	yes	71.58243	22.87009	77.21547	64.45156	12.763904
name	no	75.30308	13.76300	79.72130	69.99943	9.721863
store	yes	67.55119	61.60366	77.89089	58.24407	19.646821
store	no	68.65713	77.88680	80.92176	58.53920	22.382569

Table 10: Least Squares Means

Temp	Stirred	Mean	Var	Max	Min	Spread
6	yes	76.76972	0.8203152	77.89089	75.80973	2.081166
6	no	79.24151	0.9757520	80.92176	77.78345	3.138317
23	yes	69.44135	15.0841513	75.37855	65.92809	9.450466
23	no	71.93952	22.5021998	76.83265	67.08353	9.749120
40	yes	62.48936	14.2117017	68.08492	58.24407	9.840843
40	no	64.75929	38.5508753	71.20207	58.53920	12.662879

Table 11: Contrast Stirred and Brand

Brand	Temp	Stirred	emmean	SE	df	lower.CL	upper.CL
name	6	yes	76.20241	0.5374175	36	75.11248	77.29235
store	6	yes	77.33703	0.5374175	36	76.24709	78.42696
name	23	yes	72.69145	0.5374175	36	71.60152	73.78138
store	23	yes	66.19126	0.5374175	36	65.10132	67.28119
name	40	yes	65.85343	0.5374175	36	64.76350	66.94337
store	40	yes	59.12529	0.5374175	36	58.03535	60.21522
name	6	no	78.99061	0.5374175	36	77.90068	80.08055
store	6	no	79.49240	0.5374175	36	78.40247	80.58233
name	23	no	76.36351	0.5374175	36	75.27358	77.45344
store	23	no	67.51552	0.5374175	36	66.42559	68.60546
name	40	no	70.55511	0.5374175	36	69.46518	71.64505
store	40	no	58.96347	0.5374175	36	57.87354	60.05341

Table 12: Contrast Stirred versus Brand

contrast	estimate	SE	df	lower.CL	upper.CL
stirred	-2.413294	0.3102781	36	-3.042567	-1.784021
branding	5.338595	0.3102781	36	4.709322	5.967868

Table 13: Contrast Temperatures

contrast	estimate	SE	df	lower.CL	upper.CL
stirredbrand	-3.720646	0.4387996	36	-4.610573	-2.8307197
stirredstore	-1.105942	0.4387996	36	-1.995869	-0.2160151

contrast	estimate	SE	df	lower.CL	upper.CL
temp6_23	7.3151767	0.3800116	36	6.254195	8.3761584
temp6_40	14.3812861	0.3800116	36	13.320305	15.4422678
temp23_40	7.0661094	0.3800116	36	6.005128	8.1270910
temp6_rest	10.8482314	0.3290997	36	9.929394	11.7670685
temp23_rest	-0.1245337	0.3290997	36	-1.043371	0.7943034
temp40_rest	-10.7236978	0.3290997	36	-11.642535	-9.8048607

Table 15: Model 1: ANOVA Table

	Df	Sum Sq	Mean Sq	F value	Pr(>F)
Brand	1	342.007	342.007	296.041	0.000
Temp	2	1654.737	827.368	716.169	0.000
Stirred	1	69.888	69.888	60.495	0.000
Brand:Temp	2	231.852	115.926	100.345	0.000
Brand:Stirred	1	20.510	20.510	17.753	0.000
Temp:Stirred	2	0.125	0.062	0.054	0.948
Brand:Temp:Stirred	2	9.056	4.528	3.919	0.029
Residuals	36	41.590	1.155	NA	NA

Table 16: Model 1: Type III ANOVA Table

	Sum Sq	Df	F value	Pr(>F)
(Intercept)	23227.231	1	20105.451	0.000
Brand	2.575	1	2.229	0.144
Temp	221.582	2	95.901	0.000
Stirred	15.548	1	13.458	0.001
Brand:Temp	80.110	2	34.672	0.000
Brand:Stirred	0.400	1	0.347	0.560
Temp:Stirred	3.668	2	1.588	0.218
Brand:Temp:Stirred	9.056	2	3.919	0.029
Residuals	41.590	36	NA	NA

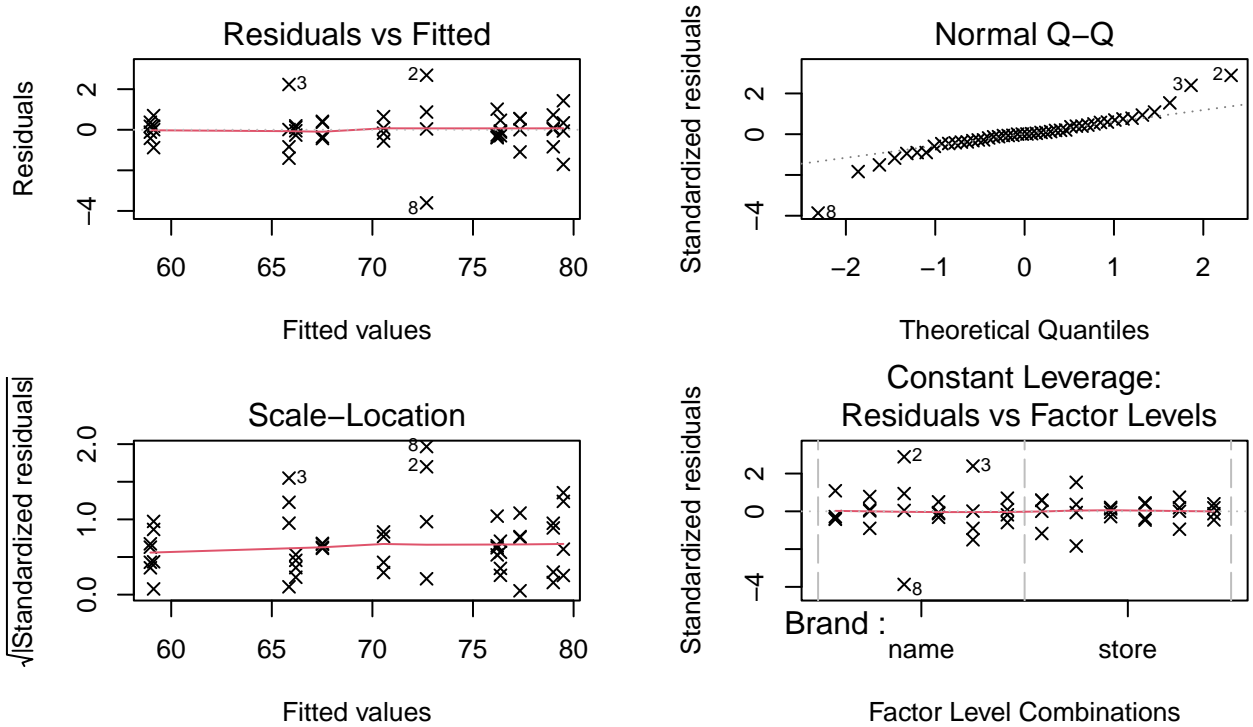


Table 17: Model 2: ANOVA Table

	Df	Sum Sq	Mean Sq	F value	Pr(>F)
Brand	1	342.00715	342.007154	196.71962	0e+00
Temp	2	1654.73655	827.368276	475.89522	0e+00
Stirred	1	69.88787	69.887866	40.19891	1e-07
Brand:Temp	2	231.85191	115.925956	66.67963	0e+00
Residuals	41	71.28061	1.738551	NA	NA

Table 18: Model 2: Type III ANOVA Table

	Sum Sq	Df	F value	Pr(>F)
(Intercept)	40014.251	1	23015.858	0.000
Brand	2.678	1	1.540	0.222
Temp	366.976	2	105.541	0.000
Stirred	69.888	1	40.199	0.000
Brand:Temp	231.852	2	66.680	0.000
Residuals	71.281	41	NA	NA

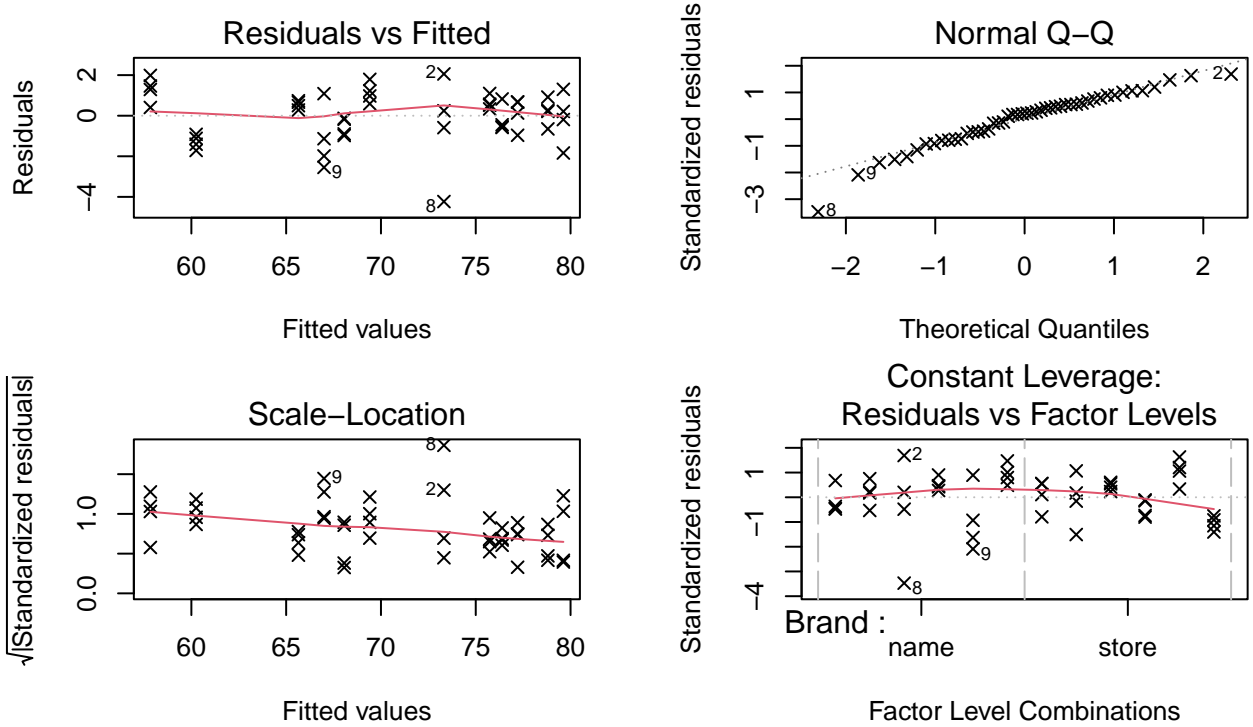


Table 19: Model 3: ANOVA Table

	Df	Sum Sq	Mean Sq	F value	Pr(>F)
Brand	1	342.00715	342.007154	48.514451	0.0000000
Temp	2	1654.73655	827.368276	117.363970	0.0000000
Stirred	1	69.88787	69.887866	9.913744	0.0029802
Residuals	43	303.13252	7.049593	NA	NA

Table 20: Model 3: Type III ANOVA Table

	Sum Sq	Df	F value	Pr(>F)
(Intercept)	60625.967	1	8599.924	0.000
Brand	342.007	1	48.514	0.000
Temp	1654.737	2	117.364	0.000
Stirred	69.888	1	9.914	0.003
Residuals	303.133	43	NA	NA

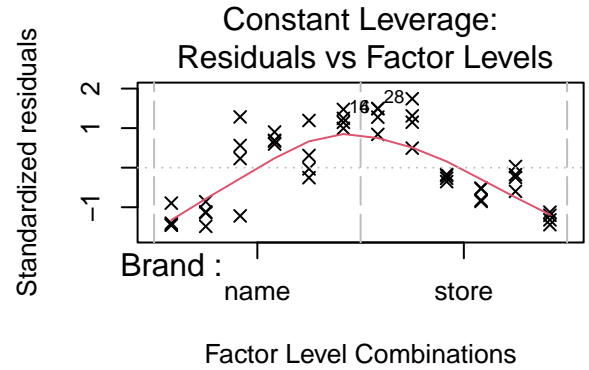
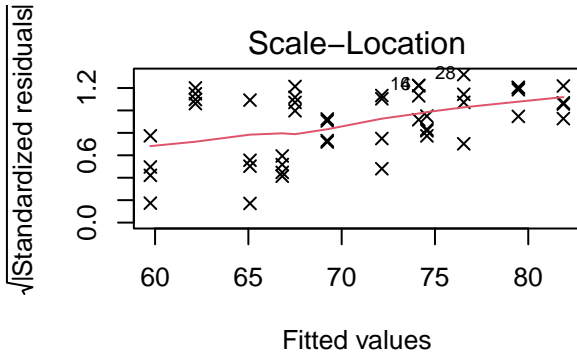
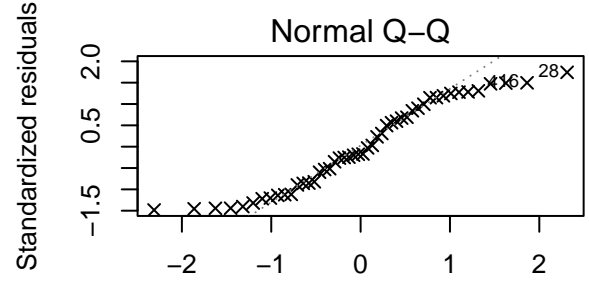
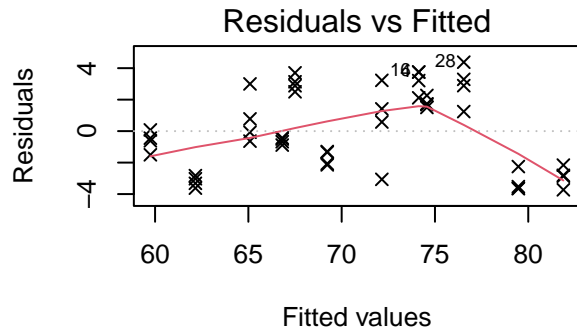


Table 21: Mixed Effects Models

Source	Df	Sum Sq	Mean Sq	Error Term	Error Df	F Score	Pr>F
Brand	1	342.0072	342.007154	MSAB	2	2.950221	0.2280
Temp	2	1654.7366	827.368276	MSAB	2	7.137041	0.1229
Brand*Temp	2	231.8519	115.925956	MSE	42	34.491507	0.0000
Residual	42	141.1685	3.361154	NA	NA	NA	NA

Table 22: Model4: Brand is Fixed and Temperature is Random

Brand	Mean	Effect
name	73.443	0.000
store	68.104	-5.339

Cov Parm	Estimate
Temp	44.465
Brand*Temp	14.071
Residual	3.361

Table 24: Model5: Brand is Random and Temperature is Fixed

Temp	Mean	Effect
6	78.006	0.000
23	70.690	-7.315
40	63.624	-14.381

Cov Parm	Estimate
Brand	9.42
Brand*Temp	14.071
Residual	3.361

Table 26: Model6: Brand and Temperature are Random

Cov Parm	Estimate
Brand	9.42
Temp	44.465
Brand*Temp	14.071
Residual	3.361

Table 27: Model 7: ANOVA Table

	Df	Sum Sq	Mean Sq	F value	Pr(>F)
Brand	1	342.0071543	342.0071543	201.4523573	0.0000000
Temp	2	1654.7365514	827.3682757	487.3444529	0.0000000
Stirred	1	69.8878657	69.8878657	41.1660257	0.0000001
Order	1	0.9059095	0.9059095	0.5336076	0.4693512
Brand:Temp	2	234.3183134	117.1591567	69.0102180	0.0000000
Residuals	40	67.9082953	1.6977074	NA	NA

Table 28: Model 7: Type III ANOVA Table

	Sum Sq	Df	F value	Pr(>F)
(Intercept)	22049.754	1	12987.959	0.000
Brand	3.577	1	2.107	0.154
Temp	335.887	2	98.924	0.000
Stirred	6.156	1	3.626	0.064
Order	3.372	1	1.986	0.166
Brand:Temp	234.318	2	69.010	0.000
Residuals	67.908	40	NA	NA

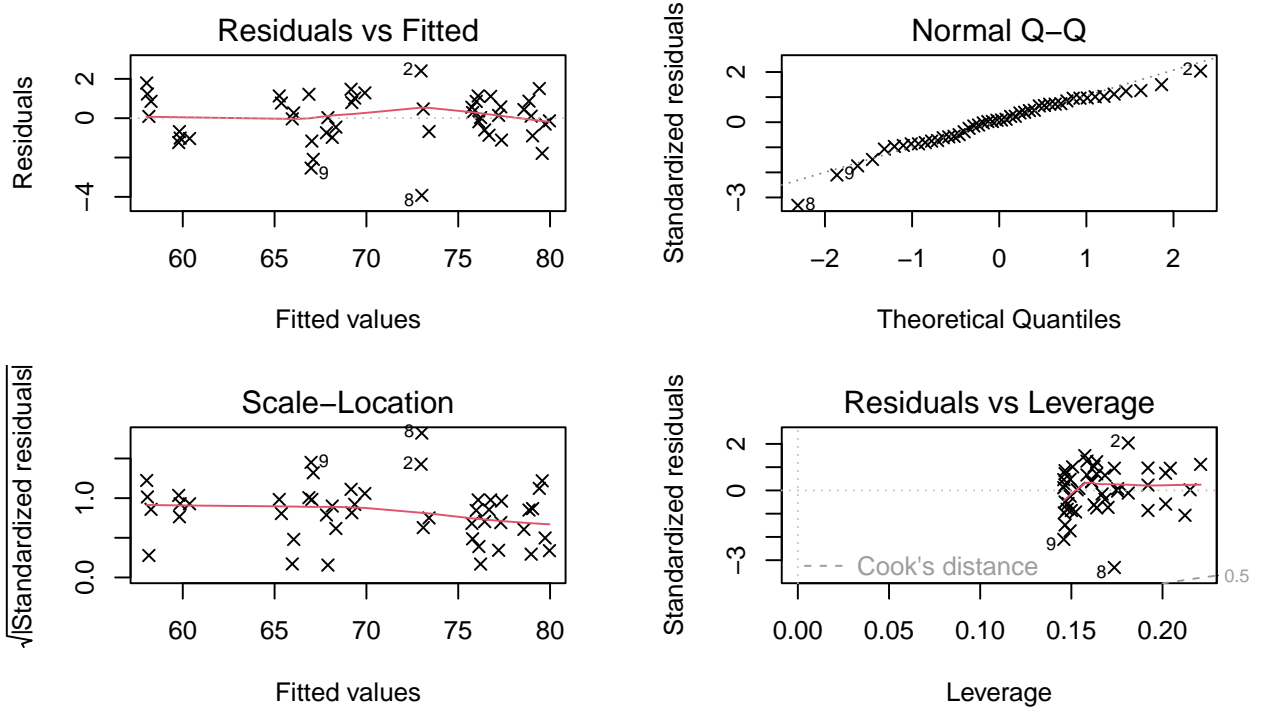
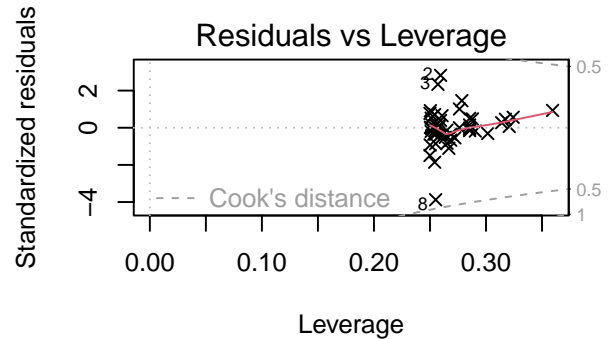
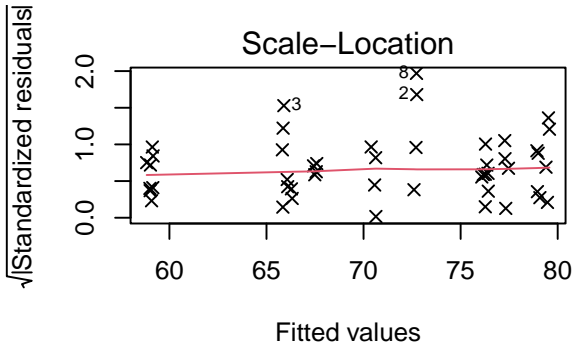
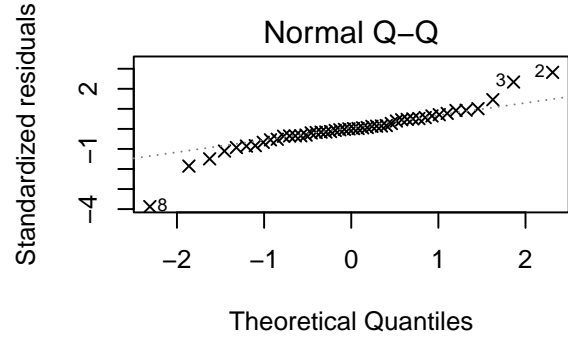
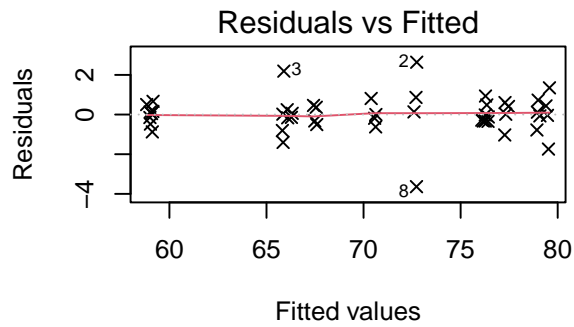


Table 29: Model 8: ANOVA Table

	Df	Sum Sq	Mean Sq	F value	Pr(>F)
Brand	1	342.0071543	342.0071543	289.5117212	0.0000000
Temp	2	1654.7365514	827.3682757	700.3736925	0.0000000
Stirred	1	69.8878657	69.8878657	59.1606229	0.0000000
Order	1	0.9059095	0.9059095	0.7668595	0.3871609
Brand:Temp	2	234.3183134	117.1591567	99.1761391	0.0000000
Brand:Stirred	1	17.2952414	17.2952414	14.6405566	0.0005144
Temp:Stirred	2	0.0420436	0.0210218	0.0177951	0.9823712
Brand:Temp:Stirred	2	9.2246692	4.6123346	3.9043772	0.0294693
Residuals	35	41.3463412	1.1813240	NA	NA

Table 30: Model 8: Type III ANOVA Table

	Sum Sq	Df	F value	Pr(>F)
(Intercept)	15086.643	1	12770.961	0.000
Brand	2.356	1	1.994	0.167
Temp	220.855	2	93.478	0.000
Stirred	9.911	1	8.390	0.006
Order	0.243	1	0.206	0.653
Brand:Temp	69.452	2	29.396	0.000
Brand:Stirred	0.409	1	0.346	0.560
Temp:Stirred	3.500	2	1.482	0.241
Brand:Temp:Stirred	9.225	2	3.904	0.029
Residuals	41.346	35	NA	NA



Appendix: Code

```
library(tidyverse)
library(emmeans)
library(lme4)
library(lmerTest)
library(olsrr)
library(car)
library(cowplot)
df_eff <- read_csv('effervescence.csv', col_types = 'fffnnn')
df_stats <-
df_eff %>% group_by(Brand, Temp, Stirred) %>%
summarise('Min' = min(Time),
          '25%' = quantile(Time, probs = 0.25),
          'Mean' = mean(Time),
          'Median' = median(Time),
          '75%' = quantile(Time, probs = 0.75),
          'Max' = max(Time),
          'Range' = Max - Min,
          'Var' = var(Time),
          'n' = n())

means_table <- df_eff %>% group_by(Brand, Temp) %>% summarise('Mean' = mean(Time))
means_table <- means_table %>% pivot_wider(names_from = Brand, values_from = Mean)
means_table$TempMean <- rowMeans(means_table[,2:3])
means_table <- cbind('Temp' = c('6', '23', '40', 'Brand Mean'), rbind(means_table[,2:4], colMeans(means_
knitr::kable(means_table, digits = 2, col.names = c("Temp", "Name", "Store", "Temp. Mean"),
              caption = "Means Table")

change_var <-
df_eff %>% group_by(Brand, Temp) %>% summarise('Mean' = mean(Time),
          'Var' = var(Time),
          'Max' = max(Time),
          'Min' = min(Time),
          'Spread' = Max - Min)

change_varplot <-
ggplot(change_var) + geom_point(aes(x = Temp, y = Var, col = Brand)) +
  geom_line(aes(x = Temp, y = Var, col = Brand, group = Brand)) +
  labs(title = "Change in Variance",
        subtitle = "Over Temperature",
        x = '',
        y = 'Variance') +
  theme(legend.position = c(0.85, 0.75),
        plot.title = element_text(size = 8, face = "bold"),
        plot.subtitle = element_text(size = 7, face = "bold"),
        axis.text = element_text(size = 7),
        axis.title = element_text(size = 8),
        legend.text = element_text(size=5, face="bold"),
        legend.title = element_text(size=6, face="bold"),
        legend.key.size = unit(0.4, 'cm'),
        legend.key = element_rect(colour = "transparent",
                                   fill = alpha("white", 0)),
                                   fill = alpha("white", 0)))
```

```

change_var2 <-
df_eff %>% filter(Stirred == "yes") %>% group_by(Brand, Temp) %>% summarise('Mean' = mean(Time),
                                     'Var' = var(Time),
                                     'Max' = max(Time),
                                     'Min' = min(Time),
                                     'Spread' = Max - Min)

change_var2plot <-
ggplot(change_var2) + geom_point(aes(x = Temp, y = Var, col = Brand)) +
  geom_line(aes(x = Temp, y = Var, col = Brand, group = Brand)) +
  labs(title = "Change in Variance",
       subtitle = "Over Temperature (Stirred)",
       x = '',
       y = '') +
  theme(legend.position = c(0.85, 0.8),
        plot.title = element_text(size = 8, face = "bold"),
        plot.subtitle = element_text(size = 7, face = "bold"),
        axis.text = element_text(size = 7),
        axis.title = element_text(size = 8),
        legend.text = element_text(size=5, face="bold"),
        legend.title = element_text(size=6, face="bold"),
        legend.key.size = unit(0.4, 'cm'),
        legend.key = element_rect(colour = "transparent",
                                   fill = alpha("white", 0)),
                                   fill = alpha("white", 0)))

change_var3 <-
df_eff %>% filter(Stirred == "no") %>% group_by(Brand, Temp) %>% summarise('Mean' = mean(Time),
                                     'Var' = var(Time),
                                     'Max' = max(Time),
                                     'Min' = min(Time),
                                     'Spread' = Max - Min)

change_var3plot <-
ggplot(change_var3) + geom_point(aes(x = Temp, y = Var, col = Brand)) +
  geom_line(aes(x = Temp, y = Var, col = Brand, group = Brand)) +
  labs(title = "Change in Variance",
       subtitle = "Over Temperature (Not Stirred)",
       x = '',
       y = '') +
  theme(legend.position = c(0.85, 0.8),
        plot.title = element_text(size = 8, face = "bold"),
        plot.subtitle = element_text(size = 7, face = "bold"),
        axis.text = element_text(size = 7),
        axis.title = element_text(size = 8),
        legend.text = element_text(size=5, face="bold"),
        legend.title = element_text(size=6, face="bold"),
        legend.key.size = unit(0.4, 'cm'),
        legend.key = element_rect(colour = "transparent",
                                   fill = alpha("white", 0)),
                                   fill = alpha("white", 0)))

plot_grid(change_varplot, change_var2plot, change_var3plot, ncol = 3)
df_eff %>% ggplot() + geom_boxplot(aes(fill = Brand, y = Time, x = Temp)) +
  facet_grid(cols = vars(Stirred)) + labs(title = "Stirred") + theme(

```

```

    plot.title = element_text(hjust = 0.5)
  )
  ##3 factor interaction plot based on HW7 code
  par(mfrow=c(2,2), mar = c(3.5,3.5,2,2))
  with(df_eff%>%filter(Stirred=="yes"),interaction.plot(Temp,Brand,Time,
    type="b", pch=20, col=c(2,4), ylab="", xlab = "",
    main="Mean Time vs. Temp: Stirred = Yes",
    cex.main = 0.75, cex.axis = 0.7, legend = FALSE))
  legend("topright",
    title = "Brand",
    c("Name", "Store"),
    bty = "n",
    cex = 0.7,
    col = c("#DF536B", "#2297E6"),
    pch = c(19,19), lty = c(2,1))
  title(xlab = "Temperature", ylab = "Mean Dissolving Time", line = 2.25, cex.lab = 0.7)

  with(df_eff%>%filter(Stirred=="no"),interaction.plot(Temp,Brand,Time,
    type="b", pch=20, col=c(2,4), ylab="", xlab = "",
    main="Mean Time vs. Temp: Stirred = No",
    cex.main = 0.75, cex.axis = 0.7, legend = FALSE))
  legend("topright",
    title = "Brand",
    c("Name", "Store"),
    bty = "n",
    cex = 0.7,
    col = c("#DF536B", "#2297E6"),
    pch = c(19,19), lty = c(2,1))
  title(xlab = "Temperature", ylab = "Mean Dissolving Time", line = 2.25, cex.lab = 0.7)
  with(df_eff%>%filter(Brand=="store"),interaction.plot(Temp,Stirred,Time,
    type="b", pch=20, col=c(2,4), ylab="", xlab = "",
    main="Mean Time vs. Temp: Brand = Store",
    cex.main = 0.75, cex.axis = 0.7, legend = FALSE))
  legend("topright",
    title = "Stirred",
    c("Yes", "No"),
    bty = "n",
    cex = 0.7,
    col = c("#DF536B", "#2297E6"),
    pch = c(19,19), lty = c(2,1))
  title(xlab = "Temperature", ylab = "Mean Dissolving Time", line = 2.25, cex.lab = 0.7)

  with(df_eff%>%filter(Brand=="name"),interaction.plot(Temp,Stirred,Time,
    type="b", pch=20, col=c(2,4), ylab="", xlab = "",
    main="Mean Time vs. Temp: Brand = Name",
    cex.main = 0.75, cex.axis = 0.7, legend = FALSE))
  legend("topright",
    title = "Stirred",
    c("Yes", "No"),
    bty = "n",
    cex = 0.7,
    col = c("#DF536B", "#2297E6"),
    pch = c(19,19), lty = c(2,1))

```

```

title(xlab = 'Temperature', ylab = "Mean Dissolving Time", line = 2.25, cex.lab = 0.7)
#model1
aov_eff <- aov(lm_eff <- lm(Time ~ Brand * Temp * Stirred, data = df_eff))

```

```

cooksD_values <- cooks.distance(lm_eff)

```

```

CD_plot <- ggplot() +
  geom_col(aes(y = cooksD_values, x = 1:length(cooksD_values)),
    width = 0.025, col = 'red') +
  geom_point(aes(y = cooksD_values, x = 1:length(cooksD_values)), shape = 20) +
  xlab('Sample Points') + ylab("Cook's Distance") +
  geom_hline(yintercept = 0.25, lty = 2) +
  labs(title = "Cook's Distance") +
  theme(
    plot.title = element_text(size = 10, face = "bold"),
    axis.text = element_text(size = 7),
    axis.title = element_text(size = 8)
  )

```

```

#CD_plot <- ols_plot_cooksd_chart(lm_eff)
qqplot1 <- ggplot(df_eff, aes(sample = Time)) +
  stat_qq(shape = 20) +
  stat_qq_line(linetype = "dashed", col = 'red') +
  labs(x = "Theoretical Quantiles",
    y = "Sample Quantiles",
    title = "Normal Q-Q Plot") +
  theme(
    plot.title = element_text(size = 10, face = "bold"),
    axis.text = element_text(size = 7),
    axis.title = element_text(size = 8)
  )

```

```

plot_grid(CD_plot, qqplot1)

```

```

#model with stirred as block effect without interaction

```

```

#model2

```

```

aov_block_eff <- aov(lm_block_eff <- lm(Time ~ Brand * Temp + Stirred, data = df_eff))

```

```

#model3

```

```

aov_block_eff_noint <- aov(lm_block_eff <- lm(Time ~ Brand + Temp + Stirred, data = df_eff))

```

```

#added covariate Order model with stirred as block effect without interaction

```

```

#model7

```

```

aov_block_order_eff <- aov(lm_block_order_eff <- lm(Time ~ Brand * Temp + Stirred + Order, data = df_eff))

```

```

#model8

```

```

aov_three_order_eff <- aov(lm_three_order_eff <- lm(Time ~ Brand * Temp * Stirred + Order, data = df_eff))

```

```

RMSE_function <- function(df_aov){

```

```

  r_mse <- sqrt(sum(df_aov$residuals^2)/df_aov$df)

```

```

  r_s <- 1 - tail(summary(df_aov)[1][[1]][[2]], n = 1) / sum(summary(df_aov)[1][[1]][[2]])

```

```

  a_r_s <- 1 - (1 - r_s)*(nrow(df_aov$model) - 1)/(df_aov$df)

```

```

  aic_ <- AIC(df_aov)

```

```

bic_ <- BIC(df_aov)

output_stats <- c(
  r_mse,
  r_s,
  a_r_s,
  aic_,
  bic_
)
return(output_stats)
}

Model1 <- RMSE_function(aov_eff)
Model2 <- RMSE_function(aov_block_eff)
Model3 <- RMSE_function(aov_block_eff_noint)
Model7 <- RMSE_function(aov_block_order_eff)
Model8 <- RMSE_function(aov_three_order_eff)

d <- rbind(Model1, Model2, Model3, Model7, Model8)
colnames(d) <- c('Root MSE', '$R^2$', 'adj $R^2$', 'AIC', 'BIC')
knitr::kable(d, escape = FALSE, digits = 3, align = "cccc")
knitr::kable(summary(aov_eff)[[1]], 'simple', digits = 3, caption = 'Model 1: ANOVA Table')
means_eff <- emmeans(aov_eff, specs = c('Brand', 'Temp', 'Stirred'))
#summary(means_eff)
cont_str_brd <-
contrast(means_eff, list(stirred = c(1/6, 1/6, 1/6, 1/6, 1/6, 1/6, -1/6, -1/6, -1/6, -1/6, -1/6, -1/6),
                             branding = rep(c(1/6, -1/6), 6)
                           )
)

cont_strbrd <-
contrast(means_eff, list(stirredbrand = c(1/3, 0, 1/3, 0, 1/3, 0, -1/3, 0, -1/3, 0, -1/3, 0),
                             stirredstore = c(0, 1/3, 0, 1/3, 0, 1/3, 0, -1/3, 0, -1/3, 0, -1/3)
                           )
)

cont_temp <-
contrast(means_eff, list(temp6_23 = c(1/4, 1/4, -1/4, -1/4, 0, 0, 1/4, 1/4, -1/4, -1/4, 0, 0),
                             temp6_40 = c(1/4, 1/4, 0, 0, -1/4, -1/4, 1/4, 1/4, 0, 0, -1/4, -1/4),
                             temp23_40 = c(0, 0, 1/4, 1/4, -1/4, -1/4, 0, 0, 1/4, 1/4, -1/4, -1/4),
                             temp6_rest = c(1/4, 1/4, -1/8, -1/8, -1/8, -1/8, 1/4, 1/4, -1/8, -1/8, -1/8, -1/8),
                             temp23_rest = c(-1/8, -1/8, 1/4, 1/4, -1/8, -1/8, -1/8, -1/8, 1/4, 1/4, -1/8, -1/8),
                             temp40_rest = c(-1/8, -1/8, -1/8, -1/8, 1/4, 1/4, -1/8, -1/8, -1/8, -1/8, 1/4, 1/4),
                             ), options=list(adjust="bonferroni")
)

lm_eff_me <- lm(Time ~ Brand * Temp, data = df_eff)
aov_eff_me <- aov(lm_eff_me)
anova_eff_me <- anova(lm_eff_me)

me_table <- as_tibble(summary(aov_eff_me)[[1]][,1:3])
me_table <- cbind('Source' = c('Brand', 'Temp', 'Brand*Temp', 'Residual'),
                  me_table,

```

```

      'Error Term' = c("MSAB", "MSAB", "MSE", "NA"))

MSA <- me_table[1, 4]
MSB <- me_table[2, 4]
MSAB <- me_table[3, 4]
MSE <- round(me_table[4, 4], 3)

a <- length(levels(df_eff$Brand))
b <- length(levels(df_eff$Temp))
n <- nrow(df_eff)/(a*b)

sigma_ab <- round((MSAB - MSE) / n, 3)
sigma_a <- round((MSA - MSAB) / (b * n), 3)
sigma_b <- round((MSB - MSAB) / (a*n), 3)

f_scores <- c(MSA/MSAB, MSB/MSAB, MSAB/MSE, NA)

error_dof <- c(rep(tail(me_table$Df, n = 2)[1], 2), tail(me_table$Df, n = 1)[1], NA)

me_table['Error Df'] <- error_dof

me_table['F Score'] <- f_scores
f_test <- round(1 - pf(me_table['F Score'][[1]],
                      me_table['Df'][[1]],
                      me_table['Error Df'][[1]]),
              4)

me_table['Pr>F'] <- f_test

se_mu <- sqrt((MSA+MSB-MSAB)/(a*b*n))

dof_app <- (MSA + MSB - MSAB)^2 / (MSA^2/(a-1) + MSB^2/(b-1) + MSAB^2 / ((a-1)*(b-1)))

CV_hat <- sqrt(sum(c(sigma_a, sigma_b, sigma_ab, MSE)))/mean(df_eff$Time)

re_table <- as_tibble(cbind(c('Brand', 'Temp', 'Brand*Temp', 'Residual'), round(c(sigma_a, sigma_b, sigma_ab, MSE), 3)))
colnames(re_table) <- c('Cov Parm', 'Estimate')
re_table$Estimate <- as.numeric(re_table$Estimate)
re_table$Portion <- round(as.numeric(re_table$Estimate) / sum(as.numeric(re_table$Estimate)), 3)
knitr::kable(re_table)
knitr::kable(df_stats, caption = "Data Summary Table")
df_eff %>% group_by(Brand) %>% summarise('Mean' = mean(Time), 'Var' = var(Time), 'Max' = max(Time), 'Min' = min(Time))
df_eff %>% group_by(Temp) %>% summarise('Mean' = mean(Time), 'Var' = var(Time), 'Max' = max(Time), 'Min' = min(Time))
df_eff %>% group_by(Brand, Temp) %>% summarise('Mean' = mean(Time), 'Var' = var(Time), 'Max' = max(Time), 'Min' = min(Time))
df_eff %>% group_by(Brand, Stirred) %>% summarise('Mean' = mean(Time), 'Var' = var(Time), 'Max' = max(Time), 'Min' = min(Time))
df_eff %>% group_by(Temp, Stirred) %>% summarise('Mean' = mean(Time), 'Var' = var(Time), 'Max' = max(Time), 'Min' = min(Time))
knitr::kable(summary(means_eff), caption = "Least Squares Means")
knitr::kable(confint(cont_str_brd), caption = "Contrast Stirred and Brand")
knitr::kable(confint(cont_strbrd), caption = "Contrast Stirred versus Brand")
knitr::kable(confint(cont_temp), caption = "Contrast Temperatures")
knitr::kable(summary(aov_eff)[[1]], 'simple', digits = 3, caption = 'Model 1: ANOVA Table')
knitr::kable(Anova(aov_eff, type=3), 'simple', digits = 3, caption = 'Model 1: Type III ANOVA Table') #
par(mfrow=c(2,2), mar = c(5,5,2,2))

```

```

plot(aov_eff, pch = 4)
knitr::kable(summary(aov_block_eff)[[1]],
  'simple', caption = "Model 2: ANOVA Table")
knitr::kable(Anova(aov_block_eff, type=3),
  'simple', digits = 3, caption = 'Model 2: Type III ANOVA Table')
par(mfrow=c(2,2), mar = c(5,5,2,2))
plot(aov_block_eff, pch = 4)
knitr::kable(summary(aov_block_eff_noint)[[1]],
  'simple', caption = "Model 3: ANOVA Table")
knitr::kable(Anova(aov_block_eff_noint, type=3),
  'simple', digits = 3, caption = 'Model 3: Type III ANOVA Table')
par(mfrow=c(2,2), mar = c(5,5,2,2))
plot(aov_block_eff_noint, pch = 4)

name_mean <- df_eff %>% filter(Brand == 'name') %>% select(Time) %>% unlist() %>% mean()
brand_fe <- df_eff %>% group_by(Brand) %>% summarise('Mean' = mean(Time), 'Effect' = Mean - name_mean)

name_mean <- df_eff %>% filter(Temp == '6') %>% select(Time) %>% unlist() %>% mean()
temp_fe <- df_eff %>% group_by(Temp) %>% summarise('Mean' = mean(Time), 'Effect' = Mean - name_mean)
knitr::kable(me_table, caption = 'Mixed Effects Models')

knitr::kable(brand_fe, digits = 3,
  caption = 'Model4: Brand is Fixed and Temperature is Random')

knitr::kable(cbind(c('Temp', 'Brand*Temp', 'Residual'),
  c(sigma_b, sigma_ab, MSE)), col.names = c('Cov Parm', 'Estimate'), caption = "")
knitr::kable(temp_fe, caption = 'Model5: Brand is Random and Temperature is Fixed',
  digits = 3)
knitr::kable(cbind(c('Brand', 'Brand*Temp', 'Residual'),
  c(sigma_a, sigma_ab, MSE)), col.names = c('Cov Parm', 'Estimate'),
  caption = "")
knitr::kable(cbind(c('Brand', 'Temp', 'Brand*Temp', 'Residual'),
  c(sigma_a, sigma_b, sigma_ab, MSE)), col.names = c('Cov Parm', 'Estimate'),
  caption = 'Model6: Brand and Temperature are Random')
knitr::kable(summary(aov_block_order_eff)[[1]],
  'simple', caption = "Model 7: ANOVA Table")
knitr::kable(Anova(aov_block_order_eff, type=3), 'simple',
  digits = 3, caption = 'Model 7: Type III ANOVA Table')
par(mfrow=c(2,2), mar = c(5,5,2,2))
plot(aov_block_order_eff, pch = 4)
knitr::kable(summary(aov_three_order_eff)[[1]],
  'simple', caption = "Model 8: ANOVA Table")
knitr::kable(Anova(aov_three_order_eff, type=3),
  'simple', digits = 3, caption = 'Model 8: Type III ANOVA Table')
par(mfrow=c(2,2), mar = c(5,5,2,2))
plot(lm_three_order_eff, pch = 4)

```