Design of Experiments Final Project
(STAT 263/363)

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1 Introduction

Phenomenon under investigation: We investigated the classic "Mentos and Coke" reaction under varying conditions. The experiment involves dropping Mentos candies into a 2-liter soda bottle, and observing the resulting soda eruption. This reaction occurs because the Mento candies catalyze a physical reaction: the aqueous form of carbon dioxide (CO_2) converts to the gaseous form, which rapidly expands and escapes the soda container (Buddies, 2012). While the reaction can occur by dropping a variety of different objects into the soda, Mentos are an optimal choice for catalyzing the reaction because the surface of the candy is covered in millions of microscopic divots and cavities (Bell-Young, 2022). The rough surface of the candy allows gaseous CO_2 bubbles to rapidly form, leading to the observed soda geyser (Buddies, 2012).

Goals and Expectations: Our goal was to investigate the Mentos/soda reaction under several different conditions, including number of Mentos used, soda temperature, and type of soda (Diet vs. Regular). We chose these conditions based on prior literature that suggests they have an important effect on the height of the geyser and amount of soda released from the bottle during the reaction. Based on the results of previous versions of this experiment, we expected to observe: (1) Higher temperatures increase the strength of the reaction; (2) More Mentos per liter of soda increase the strength of the reaction; and (3) More sugar in the soda decreases the strength of the reaction (Bell-Young, 2022). We expected there to be no interaction effects between the treatments, since we could not think about ways of how these effects together could create "new effects" on the reaction.

An additional goal of our experiment was to develop robust design for inference, while operating under technical and budgetary constraints. Specifically, we needed to perform the experiment using readily available tools (e.g. a refrigerator for cooling the soda, a regular kitchen scale for measuring the outcome) and limiting the total cost of materials to $40 or less.

2 Methods

We investigated three ($k = 3$) experimental conditions:

- Number of Mentos: 2 vs. 5
- Temperature of Soda: Room temperature vs. Refrigerated overnight
- Type of Soda: Regular Safeway Brand Cola vs. Diet Safeway Brand Cola

Each experimental condition is a factor with two levels. As a result, there are $2^k = 2^3 = 8$ different treatment combinations and we implemented a factorial design with $n = 2$ replicates.

This design was chosen to allow us to investigate all of the procedures of interest, collect replicate data, and stay under our total budgetary constraint. We did not need to implement a fractional factorial design as we only had three factors of interest and were able to carry out all necessary comparisons and replicates in a full fractional setting. We implemented a variation of a completely randomized design, in which we blocked based on the temperature of the soda and then randomized the treatments (soda type and number of Mentos) and replicates within each block. We chose this approach because we wanted to ensure, as best as possible given technical constraints, that the cold sodas were all similar in temperature. Due to constraints on where we could perform the experiment, we had to remove the cold sodas from the refrigerator, transport them to the outdoor parking lot, and then conduct the trials. It thus made sense to perform all of the cold experiments first so that the sodas would have minimal time to increase in temperature. The warm sodas were already at ambient temperature and we were not concerned about temperature fluctuations in this block.

The primary outcome of interest was the weight of the soda bottle (in grams, measured on a kitchen scale) after the Mentos/soda reaction complete and the bottle had been re-capped. Less weight indicates a stronger reaction because more soda escaped the bottle. The total mass of the 2-liter soda bottles prior to the reaction is approximately 2100g (2.1kg), based on the mass of liquid (which is approximately equal to the mass of pure water), the bottle, and cap. We discovered in the course of carrying out the experiment that the maximum weight our scale could read is 2100g; therefore, if there are small fluctuations in weight greater than 2100g, we cannot detect them and record the final weight as 2100g. An outcome mass of 2100g indicates that no soda escaped the bottle during the reaction.

We analyze the data in several ways. First, we examine the mean marginal effect due to each individual factor, ignoring the other two (e.g. temperature (ignoring soda type and number of Mentos), soda (ignoring temperature and number of Mentos), etc.). To test whether the differences in means by each treatment are significant when accounting for the other factors, we fit the following linear regression model (where T = temperature, M = Mentos, S = Soda):

$$\text{Outcome} = \beta_0 + \beta_1 \text{Treatment} + \epsilon \tag{1a}$$

$$\text{Outcome} = \beta_0 + \beta_1 \text{T} + \beta_2 \text{M} + \beta_3 \text{S} + \epsilon \tag{1b}$$

$$\text{Outcome} = \beta_0 + \beta_1 \text{T} + \beta_2 \text{M} + \beta_3 \text{S} + \beta_4 \text{TM} + \beta_5 \text{TS} + \beta_6 \text{MS} + \beta_7 \text{MST} + \epsilon \tag{1c}$$

where $\epsilon \sim N(0, \sigma^2)$. Equation (1a) is equivalent to an ANOVA with three independent variables- temperature, soda and Mentos- each using 1 degree of freedom. We additionally fit the model with a factor for replicate a vs. b, to test whether there are significant differences between the repeated measures, and a model including the order of the experiments to test for a time trend. Because we collect 16 data points total, we have sufficient degrees of freedom to test all two-way interactions and the three-way interaction.

3 Results

Figure 1a shows the Mentos used in conducting the experiment and weighing method for collecting the outcome data; Figure 1b shows all soda bottles after completion of the reactions. The raw data from the experiment are presented in Table 1. Data are presented in the order in which we conducted the experiment, blocking by temperature, and randomizing soda type and number of Mentos within each block (with two replicates per temperature/soda/Mentos combination). We made a small error in carrying out our design and inadvertently used a warm soda during the cold soda block (Treatment F, replicate a); in our planned design, treatment F should have been randomized in the block of warm sodas.

Figure 2 displays the marginal effect of each factorial treatment condition on the outcome of interest. Table 2 provides the mean outcome for each factor, averaging across levels of the other two factors, and mean difference across levels of the factor (the results of fitting model 1a three separate times on each factor). The marginal effect of temperature (ignoring soda type and number of Mentos) is a 31.4% greater decrease in mean soda weight at cold temperature as compared to warm (mean difference (warm - cold): -599.25g, 95% CI: (-819.77, -378.73)). The marginal effect of soda type is 15.9% greater decrease in soda weight using diet soda as compared to regular; the marginal effect of number of Mentos is a 12.1% greater decrease in soda weight using 5 Mentos as compared to 2; however the marginal effects for soda type and number of Mentos are not significant, as the confidence intervals for the mean change in outcome weight cross zero (Table 2). There is only a 2% difference, on average, between the a and b replicates of each treatment, which is also not statistically significant.

To test the significance of individual factors controlling for the others, we modeled the outcome as a linear function of temperature, soda type and number of Mentos (equivalent to an ANOVA model in this case) (the model presented in equation 1b). (Note that because we implemented a fully factorial design and the factors temperature, soda and Mentos are independent to each other, the coefficients do not change when we include the factors together in one model; however the standard error decreases and as a result the confidence intervals may change). In this model, all three treatment factors are significantly associated with the outcome, with temperature having the greatest effect (estimate, warm: -599.25g, $p \approx 3.1 \times 10^{-8}$), followed by soda type (estimate, diet: -277.75g, $p \approx 8.7 \times 10^{-5}$) and number of mentos (estimate, 5: -207.75g, $p \approx 9.9 \times 10^{-4}$). Including replicates in the model does not significantly change these effect estimates, and replicates are not significantly associated with the outcome (estimate, b: -32.50g, p = 0.52). Figure 3 shows a few data points with strong deviations from normality: Cold/Diet/5, Cold/Regular/5, Warm/Regular/2, Warm/Diet/2.

In the full model with all two-way and the three-factor interactions, no interaction appeared to be statistically significant (Table 3). Moreover, two of the treatments (Number of Mentos and Type of Soda) became non-statistically significant; only temperature has a significant effect on the outcome in this model.

4 Discussion

In this experiment we observed that the temperature of the soda has the greatest effect on the reaction strength: warm soda generates a significantly stronger reaction (as measured by the weight of soda remaining in the bottle at the completion of the reaction) as compared to colder soda. This is consistent with what we expected to find based on the known chemical and physical properties of the reaction. We additionally observed the Diet soda and using a larger number of Mentos increases the strength of the reaction, although with a smaller effect size than temperature; these factors are not significant when we account for interactions between temperature and the other factors.

Because we blocked on temperature, the blocking is confounded by temperature. We cannot test for a block effect independent of a temperature effect.This was an intentional design choice in order to try to maintain relative consistency in temperature throughout the cold soda trials. However, we were able to test whether there was a significant effect due to order of the experiment (e.g. a time trend) or significant differences between replicates; we found that there was no such significant effect for either ordering or replicates in our data.

Redoing the Experiment: While conducting the experiment, we noted several ways that we could improve the design and implementation. We list these issues below in an attempt to be transparent with our readers, facilitate replication of results, and improve this experiment in the future.

1. Stricter temperature control

    - We were limited in our ability to continuously control the temperature of the soda, due to lack of equipment and resources. Specifically, because we had to perform the experiment outdoors, we could not keep the "cold" sodas in the fridge continuously while performing the other trials. While we made our best effort to guarantee that cold and warm soda bottles had similar temperatures, it's likely that the last replications of the cold bottles in our experiment were slightly warmer than the first ones, since they were outside of the fridge for a longer period of time (about 15 minutes) before they were used in an experiment. If this is true, then we would expect these latter bottles to be lighter at the end of the experiment, as the reaction tends to be stronger at warmer temperatures. We tested this in our data by fitting a model including Order as a predictor, and found that it was not significantly associated with the outcome; this suggests that small increases in the temperature of the cold soda did not have a large effect on the results. In the future, we could improve on the design of the experiment by using a proper cooler to carry the bottles to the site of the experiment. Additionally, in future iterations of the experiment we could directly measure the temperature of the sodas using a thermometer to ensure the appropriate temperature was being maintained across trials.

2. Assumption that bottles all had the same weight prior to the experiment

    - Unfortunately, we did not weigh the bottles before the experiment. Implicitly, we assume that all bottles were the same weight (2,100g) at the start of the experiments. While this should be true because of industrial standardization in the production of these bottles, there could be some variation that we would not be able to measure.

3. Inability to add all Mentos at once for the extreme cases

    - For some cases, the reaction was so strong and fast that we were unable to add all the 5 Mentos immediately, and had to wait a few seconds until the soda stream had subsided somewhat. We should not expect that the effect of adding 5 Mentos sequentially and separated by a few seconds are the same in magnitude, since the kinetic energy of the reaction needs to pass a certain threshold for the soda to leave the bottle (and consequentially the weight of the bottle to decrease). In a new iteration of this experiment, we would either add less Mentos to the bottle or engineer a faster way to add all the Mentos before the reaction starts.

5 Conclusions

We implemented a full factorial design to examine the effect of temperature, soda type, and number of Mentos on the strength of the classic soda/Mento reaction. Of the three factors examined, warm temperature produces the greatest increase in mass of soda expelled from the bottle. Number of Mentos and type of soda have smaller effects, that are mostly mediated by temperature. Future experiments can improve on this design by using stricter temperature control measures, investigating different ways off measuring the strength of the experiment, and by adding Mentos to the soda using a more rapid method.

6 Appendix: Data and Figures

Temperature	Soda	Mentos	Outcome (g)	Treatment	Replicate	Order
Cold	Diet	5	1706	A	a	1
Cold	Diet	5	1623	A	b	2
Warm	Regular	5	1256	F	a	3
Cold	Regular	5	1995	C	a	4
Cold	Regular	2	2100	D	a	5
Cold	Regular	5	1974	C	b	6
Cold	Regular	2	2100	D	b	7
Cold	Diet	2	1848	B	a	8
Cold	Diet	2	1918	B	b	9
Warm	Regular	5	1332	F	b	10
Warm	Diet	5	1170	E	a	11
Warm	Diet	2	1405	G	a	12
Warm	Regular	2	1517	H	a	13
Warm	Diet	5	980	E	b	14
Warm	Diet	2	1106	G	b	15
Warm	Regular	2	1704	H	b	16

Table 1: Raw data from the Mentos/Soda experiment.

Factor	Level	Mean Outcome (g)	Difference in Mean Outcome (95% CI)
Temperature	Warm Cold	1308.75 1908.00	-599.25 (-819.77, -378.73)
Soda	Diet Regular	1469.50 1747.25	-277.75 (-653.61, 98.11)
Mentos	5 2	1504.50 1712.25	-207.75, (-598.19. 182.69)

Table 2: Marginal effects for each individual factor, averaging across levels of other factors. Difference in mean outcome and corresponding confidence intervals are the result of fitting the model in equation 1a, separately for each factor.

(a) Mentos used to catalyze experiment (left), weighing soda bottles after experiment (right).

(b) All soda bottles after completion of experiment.

Figure 1: Materials and experimental conditions for Mentos/soda experiment.

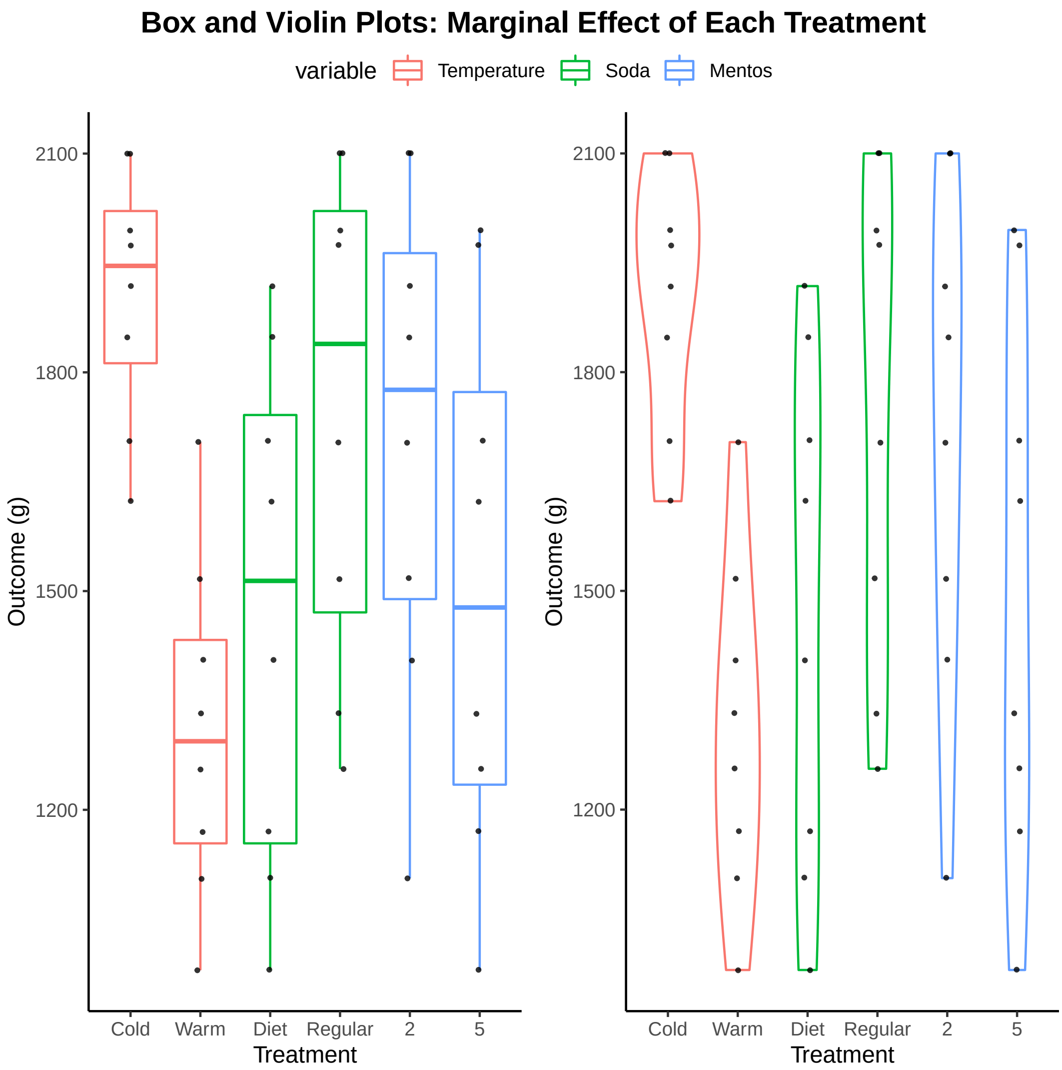

Figure 2: Box plot (left) and violin plot (right) for marginal effect of each factorial treatment (temperature: cold vs. warm, number of Mentos: 2 vs. 5, soda type: regular vs. diet) on the outcome (weight of soda bottle in grams at completion of reaction).

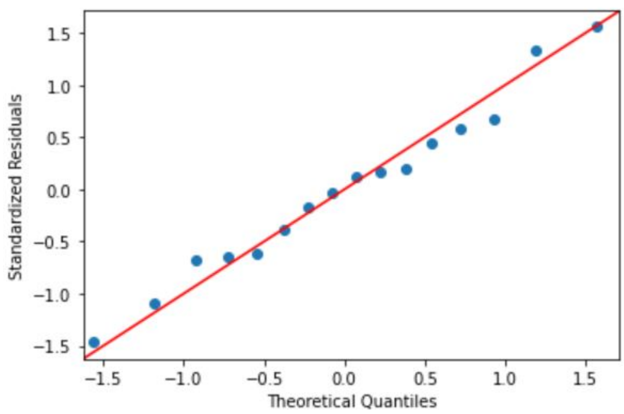

Figure 3: QQ Plot for the standardized residuals of each experiment and the theoretical quantiles for the Normal distribution.

Factor	**Reference Level**	**Model Specification**	**Coefficient [g] (95% CI)**
Temperature	Warm	1b 1c	-599.25 (-703.92 -494.58) -489.50 (-733.05, -245.95)
Soda	Diet	1b 1c	-277.75 (-382.42, -173.08) -217.00 (-460.55, 26.55)
Mentos	5	1b 1c	-207.75 (-312.42, -103.08) -115.50 (-359.05, 128.05)
Temp*Mentos	Warm, 5	1b 1c	NA -201.00 (-545.43, 143.43)
Temp*Soda	Warm, Diet	1b 1c	NA -138.00 (-482.43, 206.43)
Soda*Mentos	Diet, 5	1b 1c	NA -103.00 (-447.43, 241.43)
Temp*Soda*Mentos	Warm, Diet, 5	1b 1c	NA 239.00 (-248.10, 726.10)

Table 3: Coefficient estimates (in grams) and corresponding 95% confidence intervals for the linear model including all three main effects (model 1b) and the model including all main effects, two factor interactions, and the three-way interaction (model 1c).

7 References

Bell-Young, L. (2022, January 25). Why do mentos react with Coca-Cola? ReAgent Chemical Services.

Buddies, S. (2012, June 14). Spurting science: Erupting diet coke with Mentos. Scientific American.