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DEPARTMENT OF CHEMICAL ENGINEERING

SOCIAL TIPPING POINTS ANALYZED USING AN ECONOCHEMICAL APPROACH

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ABSTRACT

The purpose of this thesis is to introduce a new model for predicting social behavioral tipping points. Information theory, first introduced by Claude E. Shannon, suggested that analogies can be drawn between chemical phenomena and social actions observed in the physical world. This model will integrate concepts from social psychologists such as Sakoda, Schelling, and Granovetter, with the chemical phenomena of micellization and cooperative binding. These concepts were applied to the mask-wearing problem that has developed since the beginning of the SARS-CoV2 pandemic. Mask-wearing data was processed to analyze how people make decisions based on their surroundings, analogous to how molecules interact based on surroundings. Additional data about the perceptions of the population in question was used to test the stability and versatility of the model. It was found that this mask-wearing model was able to accurately predict the outcome of mask-wearing decisions $74.68 \pm 0.48\%$ of the time with a 90% confidence interval, and was most effective when the group size was larger than 2. Further extensions and refinements of the model are also discussed to evaluate how this model can be used to provide insight into different populations.

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Chapter 1

Introduction

Econochemistry is a framework centered around using chemical engineering ideas to model economic concepts, such as human social behavior, decision making, and game theory.

Econochemistry hypothesizes that humans behave like chemical systems, and make decisions similar to how chemical species react in a reactor. Previous work in the field has utilized a Chemical Game Theory model to predict how players will solve strategic games, such as Prisoner's Dilemma-type games[1]. The Chemical Game Theory model seeks to offer an alternative solution from Classical Game Theory, which solves the strategic game for how the players *should* act, assuming they are rational players. Instead, the Chemical Game Theory model does not assume players are rational, and considers player pre-biases, existing relationships, and affinities towards certain outcomes in order to predict how players *will* act. Additionally, a process control learning model of Chemical Game Theory has been analyzed to model how players update their strategies when playing repetitive games[2].

This framework has been used to hypothesize human behavior in a game setting, but has yet to address how people may act in a real-life setting, when other factors are at play. The key question that will be analyzed in this thesis is:

Does cooperative binding, as seen in the micellization of surfactant molecules, explain human decision making related to mask-wearing during the SARS-CoV-2 Pandemic?

This question will be answered by using a predictive model derived from the spontaneous interactions between surfactants to form a micelle. This model will then be compared to observed mask-wearing data collected over a period of several weeks, to determine if the chemical model accurately predicts the outcomes of the data collection. Further applications and implications will also be discussed to recommend and predict how the Econochemistry framework can be used to answer similar questions in the future.

Chapter 2

Background Chemistry

2.1 Surfactant and Micelle Chemistry

On the atomic level, a surfactant is an amphiphilic molecule with a hydrophilic head group and a non-polar hydrocarbon tail group, or chain. When placed in water or any polar solvent, these molecules spontaneously interact and form sealed bubbles, such that the hydrophobic tails are on the inside, away from the water, and the hydrophilic heads are interacting with water. This is due to the hydrophobic effect. These sealed bubbles are called micelles.

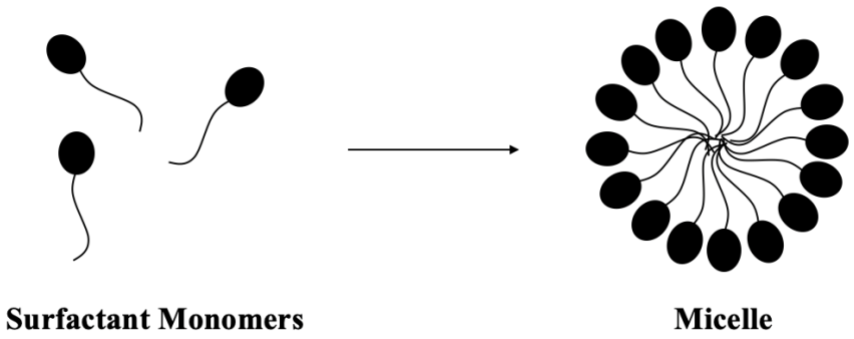
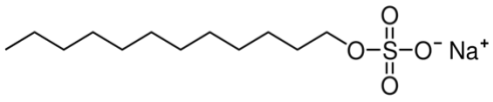
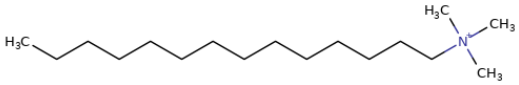
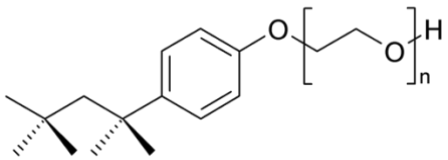


Figure 1. Depiction of surfactant to micelle formation

Initially, at a low enough concentration of surfactants, micelles do not form, because there is not enough interaction between the individual surfactants. However, at or above a specific concentration, called the critical micelle concentration (CMC), the micelles spontaneously form. Micellization is affected by several factors including surfactant chain length

and the degree of polarity of the surfactant's head groups. The following are examples of surfactants and their corresponding CMCs[3].

Table 1. Surfactant and CMC Examples

Compound Name	Compound Structure	Description	CMC (mM)
Sodium dodecylsulfate		Anionic 12-C chain	8.20
Tetradecyltrimethyl ammonium bromide		Cationic 14-C chain	3.60-3.72
Triton X-100		Non-polar Short, bulky chain	0.24-0.27

The CMC varies due to the type of surfactant in question, as well as other salts or binding agents dissolved in solution. A longer chain length will decrease the CMC, as well as the addition of electrolytes to ionic surfactants. A longer hydrocarbon chain on a surfactant would decrease the CMC because it is more favorable to form a micelle when the hydrophobicity is higher.

2.2 Cooperative Binding

Cooperative binding occurs when the number of binding sites for a ligand is a nonlinear function of its concentration, where at a specific concentration of ligands, binding occurs more rapidly[4]. This phenomenon is observed when the affinity of a ligand to a binding site is dependent on the amount of ligand already bound.

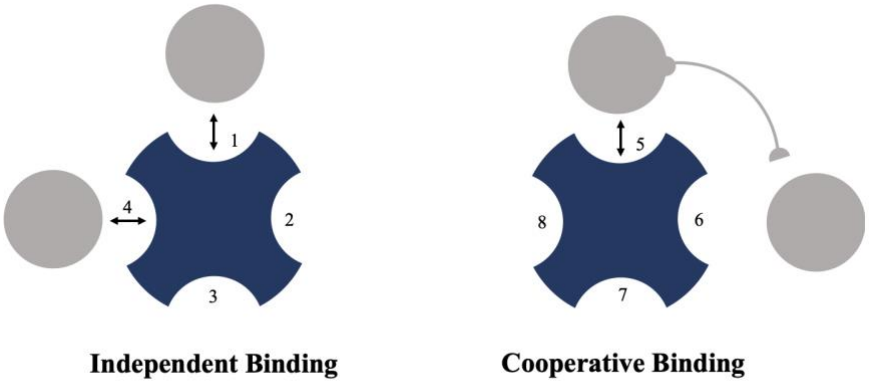


Figure 2. Independent vs Cooperative Binding

During independent binding, as seen in the ligands binding to sites 1 and 4 in Figure 2, binding site saturation is a linear function of ligand concentration, such that a larger concentration of ligands will yield a proportionally larger saturation of bound sites. During cooperative binding, the binding of one ligand increases the affinity for the next ligand to bind, as seen in the ligand in Figure 2 binding to site 5 assisting the ligand binding to site 6.

The cooperative nature of ligand binding can be positive or negative, where a bound ligand can increase or decrease the affinity for an adjacent ligand to bind. Cooperative binding is most commonly observed in proteins, which by chemical nature has numerous possible binding

sites within the quaternary structure. It is a transfer of information from one ligand to another, and the transfer of knowledge is done energetically through Gibbs free energy, G.

The binding of hemoglobin to oxygen is a common example of cooperative binding, studied by Christian Bohr in the early 1900s. Bohr found that when the hemoglobin saturation with oxygen was plotted against the partial pressure, or concentration by relation, of oxygen, an "S-shaped", or sigmoidal, plot was observed. Essentially, this observation states that as more oxygen binds to hemoglobin, it becomes easier for even more oxygen to bind. The curve then plateaus as all binding sites are saturated.

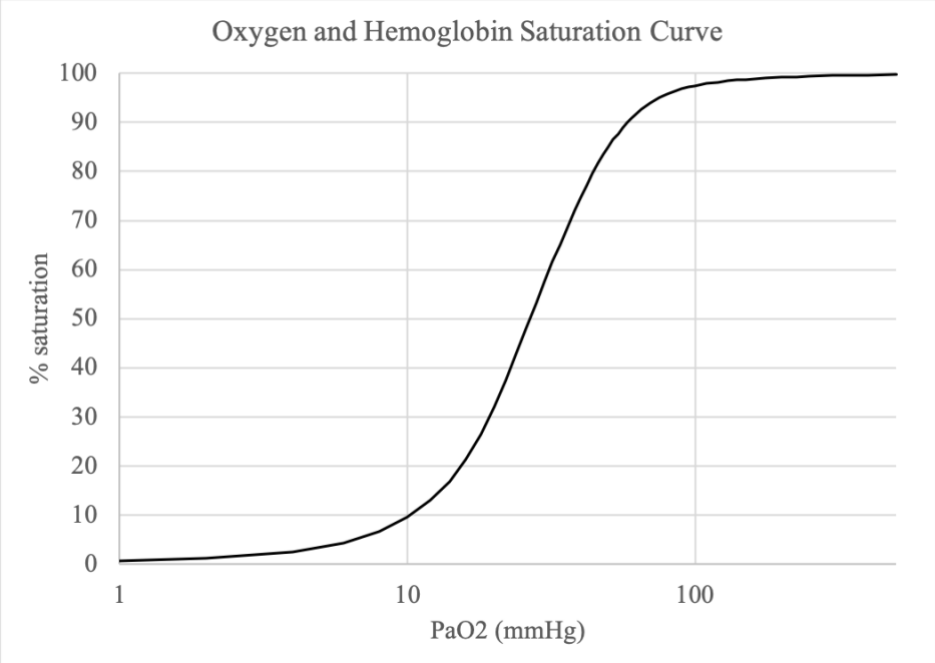


Figure 3. Sigmoidal relationship between hemoglobin binding to oxygen as a function of partial pressure of oxygen

This figure reveals the "S-shaped" curve as observed by Bohr[5], and shows that the binding of the ligand, oxygen, to the receptor molecule, hemoglobin, scales nonlinearly as ligand

concentration increases[5,6]. The fractional occupancy,θ, is defined as the quantity of binding sites that are bound by ligands divided by the total number of binding sites, which is made up of both bound and unbound sites.

$$\theta = \frac{[bound\ sites]}{[bound\ sites] + [unbound\ sites]} \qquad (1)$$

A fractional occupancy of 0 indicates the receptor molecule has no ligands bound to it and is completely unbound, while a fractional occupancy of 1 indicates complete saturation of ligands[4].

Cooperative binding operates under the assumption that ligand binding to one site directly affects the binding of a different ligand to another site. If this is not the case, then the interaction is referred to as noncooperative binding.

Cooperativity in ligand-receptor binding can be due to three-dimensional interactions, known as allosteric cooperativity. Binding sites are shaped in such a way that only certain ligands can fit properly into the site, and therefore the ligand is thermodynamically drawn to the site. Allosteric cooperative binding can be regulated positively or negatively by effector molecules that bind to the ligand and alter its conformation.

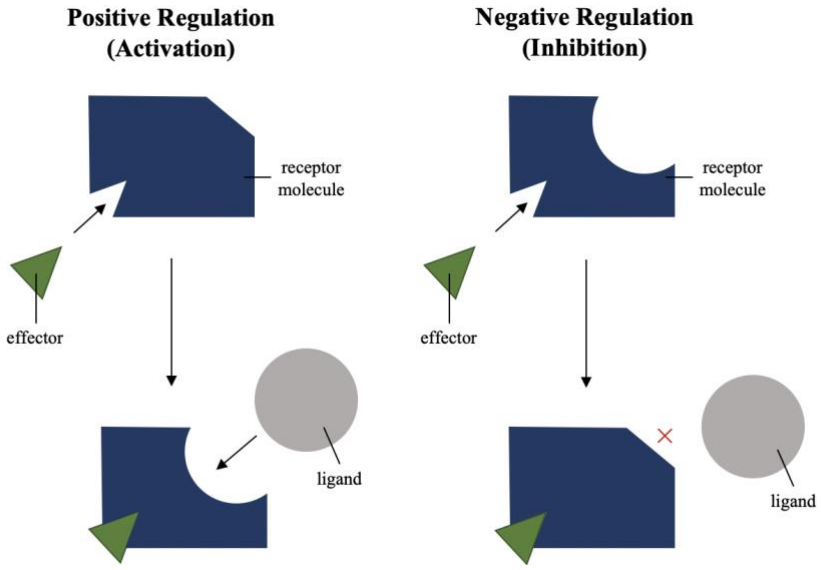


Figure 4. Positive and Negative Regulation

Positive regulation occurs when the effector molecule increases the activity of the ligand, or changes the conformation of the receptor in such a way that it is more thermodynamically favorable for the ligand to bind to the receptor. Negative regulation occurs when the effector molecule acts as an inhibitor, and changes the shape of the binding site such that the ligand cannot bind to the receptor.

Chapter 3

Social Behavior and Tipping Points

3.1 Collective Behavior and Social Tipping Points

In sociology, collective behavior is used to describe the set of actions taken within large groups of people. A "tipping point" describes a point in time when a series of smaller actions is able to cause a larger overall change. Socially, a tipping point occurs when enough individuals are engaging in a certain action to cause the rest of the population to change and engage in that same action.

Over the past few decades, models have been developed to describe collective behaviors and tipping points analytically. One of the first classical behavioral network models was introduced by Sakoda in the 1940s. Sakoda analyzed the behavior and movement within a network of individuals who have different attitudes of attraction, repulsion, and neutrality in relation to one another. The individual evaluates the positive or negative information provided from its surroundings and moves to a more preferential location in the network, such that it is closer to more positive/attractive attitudes[7].

Thomas Schelling described the world as a two-dimensional checkerboard in his 1971 paper *Dynamic Models of Segregation*[8]. He discussed how inhabitants of communities perceive their communities based on its racial composition, and move to locations on that checkerboard that meet their satisfactory composition. Schelling's model analyzes the social behavior that people attempt to avoid the minority status, and that even moderate mindsets can result in massive community segregation. This is a type of social tipping point that a population can

reach, where a certain level of minority status can cause a dramatic shift. Schelling's model has become a foundational source in many research fields such as clustering, social phase transitions, and spontaneous order and structure[9].

Social tipping point models were further developed by sociologist Mark Granovetter. His model states that people behave with a certain threshold for action, and are influenced by the number of people already acting around them. Granovetter also discusses the importance of recognizing relationships and social networks as factors that influence social tipping points. In his 1978 paper *Threshold Models of Collective Behavior*[10], the "action" in question was participation in a riot. This threshold is defined as a distribution, *f(x)*, with a cumulative distribution function, *F(x)*, for a population of *N*. The distribution function can vary based on the population at hand.

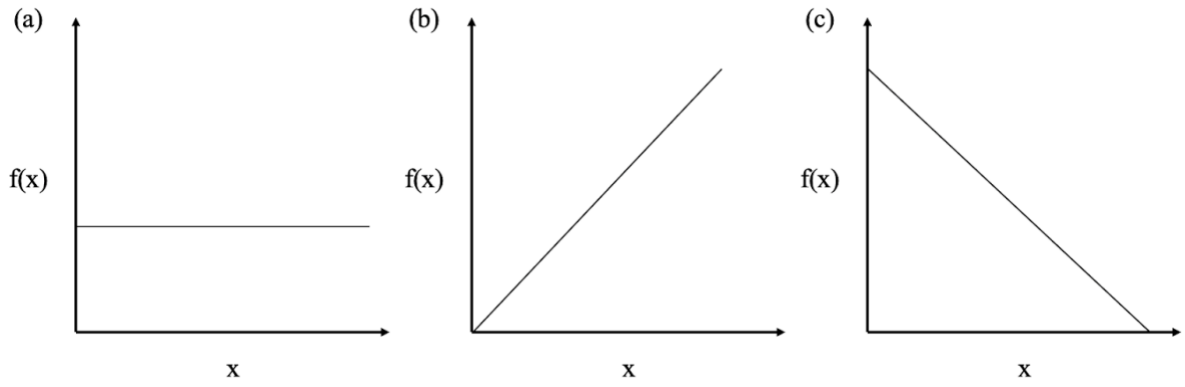


Figure 5. Depiction of three potential distribution curves (a) uniform, (b) linear increasing, and (c) linear decreasing

As seen in figure 5a, a uniform threshold distribution implies that there is an equal fraction of each threshold in the population. In a population of 100 people, the fraction is 0.01 each for a threshold of 0, 1, 2, all the way to 99. Figure 5b, a linear distribution, describes a

population with a higher fraction of people that have a higher threshold, meaning it will take more people rioting to cause the population to tip. Figure 5c, inversely, has a higher fraction of people with a lower threshold, meaning this population would riot sooner, as it takes less rioters to cause the population to tip.

Granovetter further defines the threshold model to include *R(t)*, or the number of rioters at time *t.* The number of rioters at the next time period, or *t+1*, then depends on the cumulative threshold of the previous time period as well as the population size, yielding the equation:

$$\Delta R(t+1) = NF[R(t)] \quad (2)$$

Equation 2 yields the change in the number of rioters over each time period, R(t), and when aggregated it reveals the overall collective behavior of a population, defined by a given threshold distribution F(x). The following figures display the equilibrium outcome for the populations previously defined in figure 5. These equilibriums occur when the threshold functions in figure 5 are substituted into equation 2 and solved. The slope of the distributions in figure 5b and 5c depend on the population size *N*.

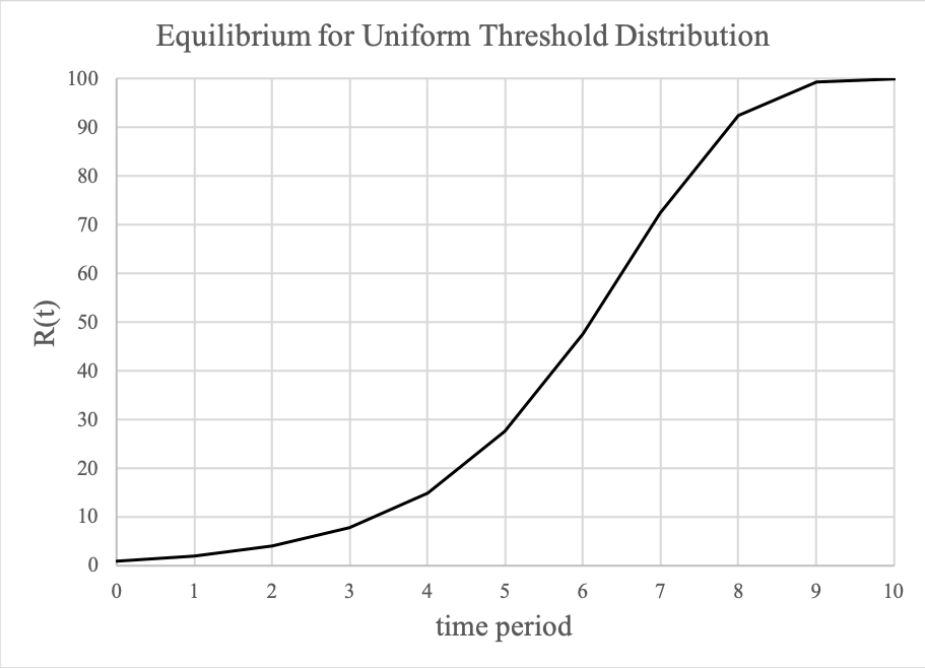


Figure 6. Equilibrium outcome for Granovetter's uniform threshold distribution

Figure 6 above that shows the equilibrium solution for the uniform threshold distribution shows a sigmoidal accumulation of riot participants over 10 time periods. It shows a relatively gradual tipping point, since there is not a singular time period that yields an overwhelming majority of rioters.

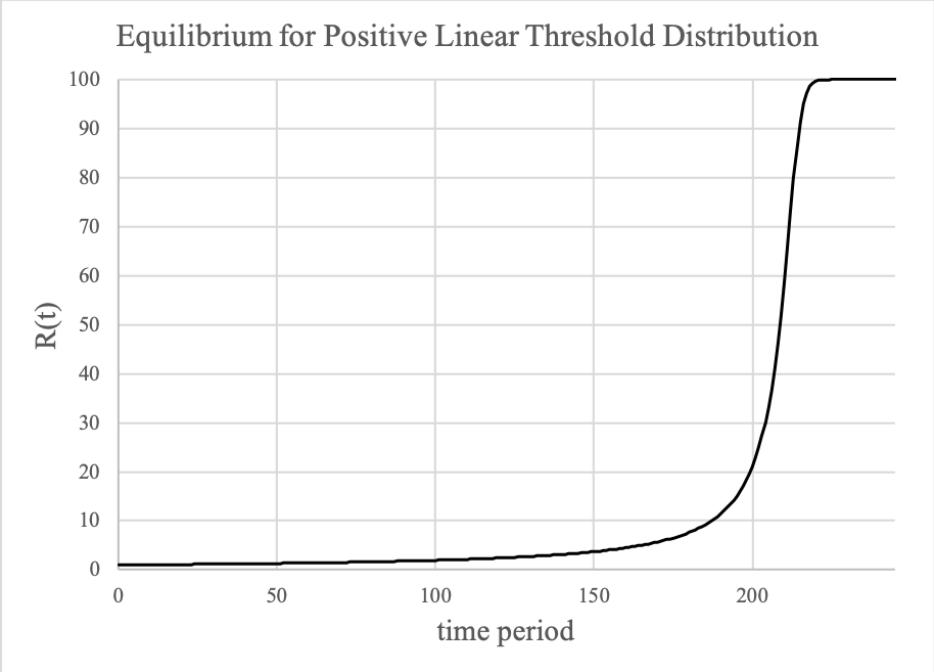


Figure 7. Equilibrium outcome for Granovetter's positive linear threshold distribution

The equilibrium for the positive linear threshold distribution reveals that it takes a significantly longer amount of time - almost 20 times as long - for this population to begin to accumulate rioters. This is because in this population, there are more people with a higher threshold, which equates to a higher resistance to riot.

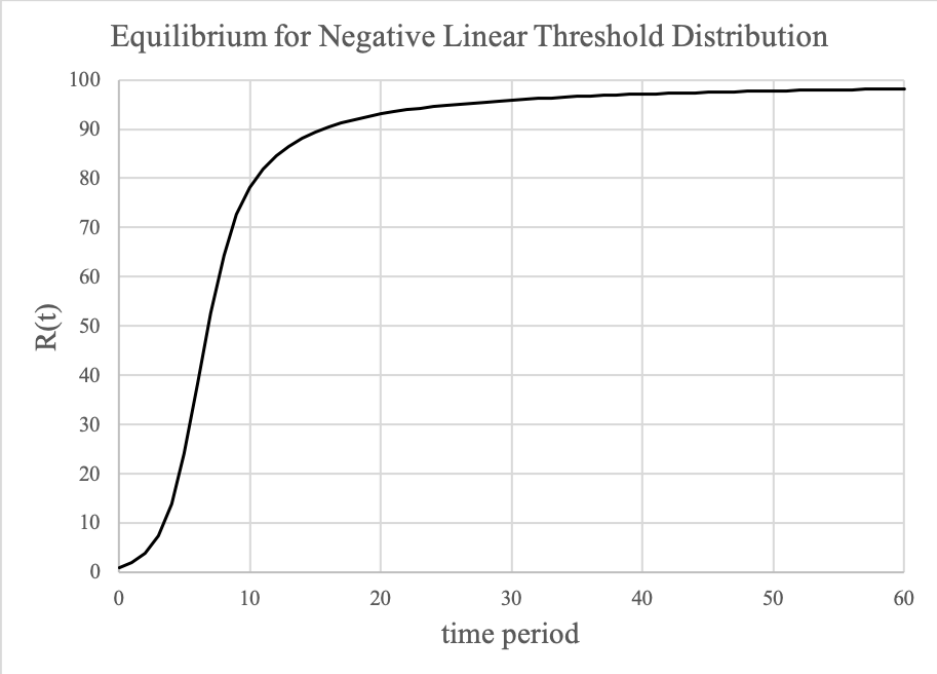


Figure 8. Equilibrium outcome for Granovetter's negative linear threshold distribution

Lastly the equilibrium for the negative linear distribution shows that a majority of the population joins riot in the first 10 time periods out of 60. However, it takes longer for the entire population to join in on the riot compared to the uniform distribution because there is still a small portion of people with a high threshold.

More recent research in the field of social tipping points analyzes tipping points in social convention. This research, done by Centola et al., uses experimental data to observe how groups of people initiate social change to establish a new equilibrium[11]. The study used actors as a portion of their participants, who acted as a "committed minority" that attempted to overthrow a previously defined social convention by introducing a new alternative. The size of this committed minority varied from about 15%-35% of the population and the equilibrium that the group reached was altered as a result. The "critical mass", which is the fraction of people in the

group that were a part of this committed minority that caused the entire group to “tip” and choose the alternative convention, was found to be about 25%. This shows that it actually doesn’t take a simple majority to have an entire population change ideas. Instead, people’s actions can be influenced by a smaller committed minority.

Sakoda, Schelling, Granovetter and Centola et al. have made huge strides in the field of social tipping points and threshold models, but certain elements can be added to these threshold models to help further define each population. Sakoda first introduced the idea of social and spatial organization, and how the attitudes surrounding an individual can impact their decision, but didn’t find a tipping point within these social interactions. The threshold models have loose definitions of the makeup of each population, such as a simple uniform or linear threshold distribution as Granovetter defines, or the positive, negative, and neutral attitudes that Sakoda defines. The calculation of the social tipping points can be refined to include more information about the population such as external factors and details about the population demographics, all of which can influence decision making but have not yet been considered.

3.2 Chemical Tipping Points

Similar to a social tipping point, a chemical tipping point occurs when a chemical species reaches a certain threshold of temperature, pressure, concentration, etc., for it to spontaneously change states or configurations. A state change is an example of a tipping point because once a substance receives or loses enough energy in the form of heat, the intermolecular forces of its molecules are altered and change configuration. The critical micelle concentration (CMC) is

considered a tipping point for micellization. At or above this concentration of surfactants, micelles spontaneously form.

The Hill-Langmuir equation is a biochemical model to describe cooperative binding as the fraction of binding sites on a macromolecule that are bound by ligands as a function of free ligands in solution[12]. It can be derived by first setting up an equilibrium equation for a receptor, *P*, with *n* number of binding sites for ligands, *L*, to bind.

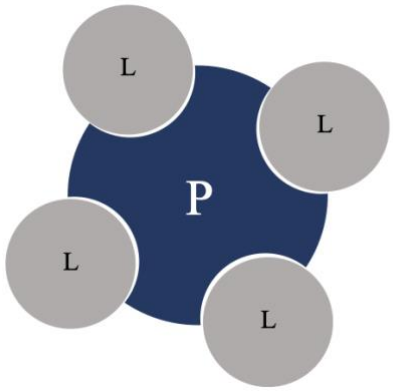


Figure 9. Receptor molecule with binding sites

$$nL + P \rightarrow PL_n \qquad (3)$$

Next, the association equilibrium constant, *K*, can be written as

$$K = \frac{[PL_n]}{[P][L]^n} \qquad (4)$$

The Hill-Langmuir equation evaluates the fraction of binding sites that are occupied by ligands, so this is expressed as a ratio of the number of bound sites to the total number of sites, as described previously in equation 1.

$$\theta = \frac{[PL_n]}{[PL_n]+[P]} \qquad (5)$$

When *[PL$_n$]* in equation 5 is replaced with the rearranged form of equation 4 and reduced by *[P]*, the following is found:

$$\theta = \frac{K[L]^n}{K[L]^n+1} \qquad (6)$$

Finally, the dissociation constant, K_d, which is simply the inverse of the association constant, *K*, is substituted into equation 6 when the entire equation is divided through by *k.*

The final form of the Hill -Langmuir equation is expressed as:

$$\theta = \frac{[L]^n}{K_d+[L]^n} \qquad (7)$$

Where is the fraction of sites bound by the ligand, *[L]* is the concentration of free, unbound ligand, K_d is the dissociation constant, and *n* is the Hill coefficient. The Hill-Langmuir equation reveals that cooperative binding of ligands experience a tipping point, which varies depending on the dissociation constant. An equivalent form of the Hill equation can be written with the association constant.

$$\theta = \frac{K[L]^n}{1+K[L]^n} \qquad (8)$$

Positive cooperativity is observed when n>1, and negative cooperativity is observed when n<1. The Hill equation also assumes that cooperativity is fixed[4].

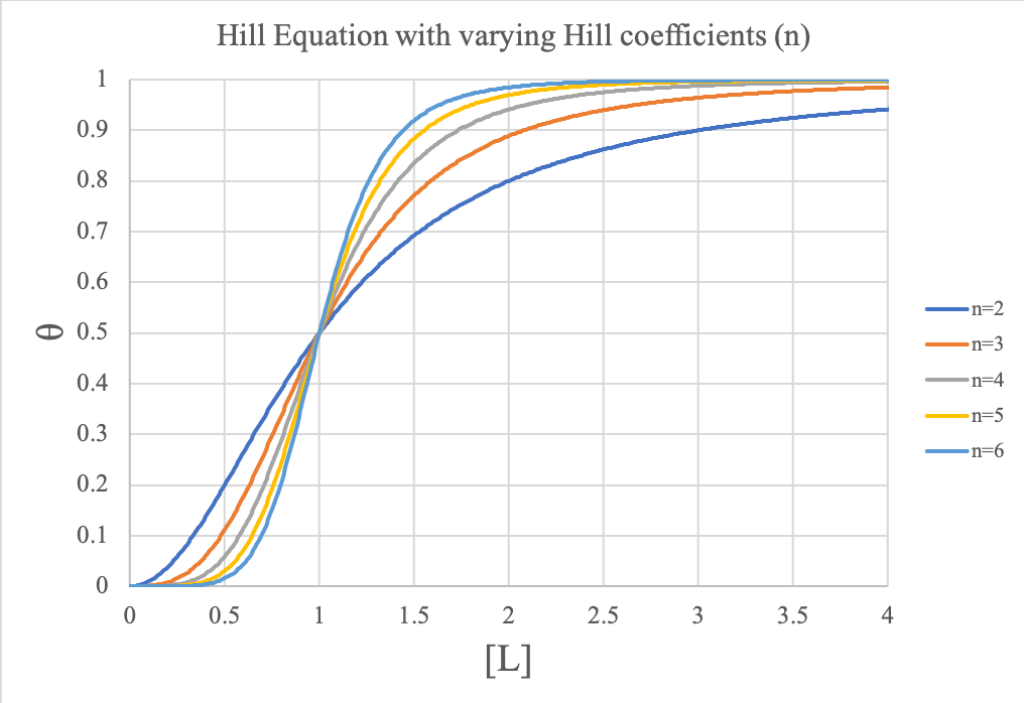


Figure 10. Graphical representation of the Hill equation with varying Hill coefficients

As seen in the plot above, as *n* increases, the tipping point, or the point at which θ increases the most dramatically with increasing *[L]*, also increases. If *n* is increased to a certain extent, then the tipping point could be achieved almost instantaneously.

3.3 Shannon Entropy and Information Theory

The model proposed in this paper aims to further define threshold models in social science by introducing a new definition in chemical terms. The idea that the physical world can be described by chemical phenomena was first introduced by Claude Shannon, an American mathematician known as “the father of information theory”. Information theory is the study of the storage and communication of information and messages. Shannon states that the semantic aspects of a message are irrelevant, and that the fact that a message is selected from a group of

possible messages is much more significant in an engineering mindset. The *Shannon Information*, or *Shannon Entropy*, of a piece of information, or message, is:

$$S_S = -k \sum_i p_i log(p_i) \qquad (9)$$

Where p_i is the probability that a message will be sent, and k is a constant to adjust for the unit of measure. This value represents how much "choice" there is in the random selection of a message with probability p_i[13] .

Chemical entropy, as defined in thermodynamics, is associated with the molecular disorder or randomness of a system. Gibbs entropy, which describes the entropy of a system with a finite number of states, is defined as:

$$S_G = -k_B \sum_i P_i ln(P_i) \qquad (10)$$

Where k_B is a thermodynamic constant also used for the unit of measurement, and P_i is the entropy of each individual microstate. The similarity between Shannon entropy in information theory and Gibbs entropy in thermodynamics is the foundational principle behind a new emerging field. There is a clear connection between phenomena that occur on an atomic scale and social interactions that involve communication and the transmittal of messages. This thesis applies the idea of information theory by using chemical phenomena to quantify and predict social behaviors.

Chapter 4

The Model and the Hypothesis

4.1 The Analogy

The formation of a micelle can be treated as a chemical reaction, with a varying number of surfactants acting as the reactants, and the micelle representing the product. This micellization can be written as a chemical equation, where reactants are driven by some equilibrium constant, *k*, to form products. In this form, it is written as:

$$nS \rightarrow M \qquad (11)$$

Where *n* represents *n* number of surfactants, *S*, that form the micelle, or product, *M*. In a similar form, the formation of ligand-receptor complexes via cooperative binding can also be treated as a chemical reaction, with a receptor molecule, *P*, and the corresponding number of ligands, *X*, representing the reactants, and the fully saturated ligand-receptor molecule representing the product.

$$nX + P \rightarrow PX_{n.} \qquad (12)$$

4.2 The Mask Wearing Model

This model hypothesizes that people behave like ligands in social decision-making situations. The surfactant-micelle model implies a certain level of spontaneity and self-assembly, where a micelle suddenly forms when the surfactant concentration reaches a certain point. The

cooperative binding model instead offers a leader-follower approach, where the "decision" of one ligand affects the "decision" of the next. As studied by Granovetter and Centola et al, people's behavior reaches a "tipping point" when enough people initiate a certain action, such that the entire group agrees to cooperate. This is much like how surfactants behave, as seen in the Hill equation and corresponding plots. At a certain concentration of ligands, the fraction of bound ligands reaches a tipping point, and the remaining ligands quickly bind until saturation is reached.

This same type of thinking was applied to the mask-wearing problem at the forefront of the SARS-CoV-2 pandemic. Although current guidelines and research encourage and often mandate wearing facial coverings in public spaces, it has been seen that not everyone complies with these regulations[14]. When individuals are alone or in small groups, they tend to wear masks much less frequently, but at a certain threshold, they are much more inclined to put their masks on. If people are treated as ligands, then what is it that causes someone to wear a mask?

In this analogy, non-mask wearers are unbound ligands, and mask-wearers are fully formed ligand-receptor complexes. The number of binding sites on the receptor molecule is equivalent to the number of people in each observed group. There are allosteric modulators, or effector molecules, that exist in solution with these ligands in the form of social and internal "reminders" such as trust in those surrounding the individual, general health and well-being of the individual, the location of the individual, and other verbal reminders and consequences that could increase the likelihood that a person will make the decision to put on their mask. These allosteric modulators are a key part of the analogy and model because in a high enough concentration of reminders, the modulators will bind to their activation site, which then changes

the conformation of the binding sites. The altered conformation allows the ligand to bind, which represents a person putting on their mask. This is analogous to an individual receiving enough information to change their decision from not wearing a mask to wearing a mask. When the concentration of allosteric modulators is low, there are not enough in solution to locate and bind to their activation sites, so the conformation of the binding sites is not changed and the ligands cannot bind. This is analogous to an individual not receiving enough information to change their decision from not wearing a mask to wearing a mask, and therefore they continue to not wear a mask.

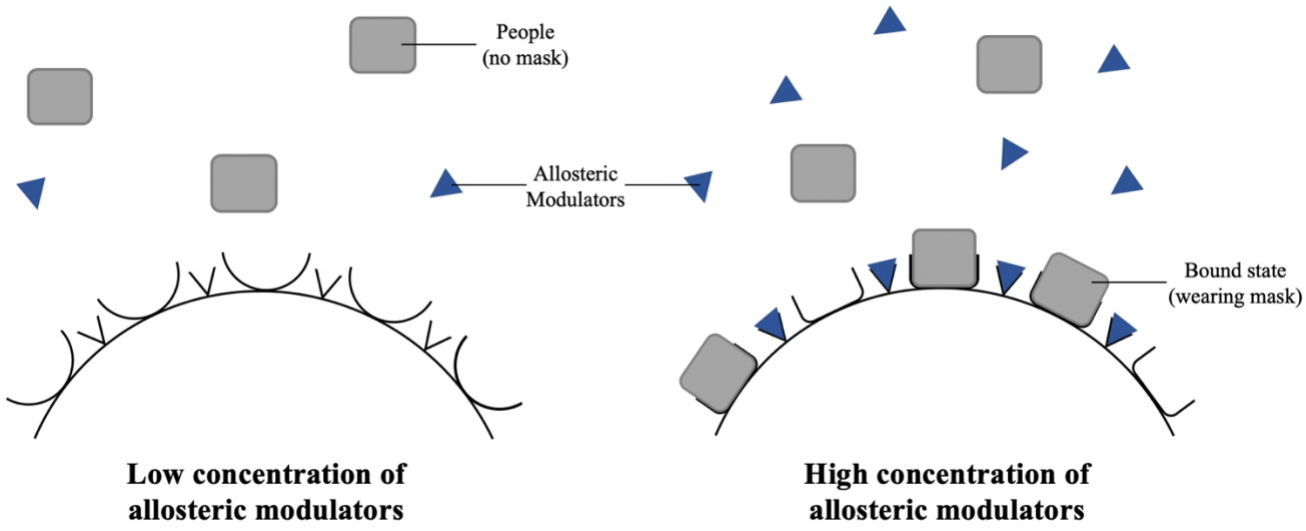


Figure 11. Allosteric regulation analogy to mask wearing

For cooperative binding, the Hill equation states that:

$$\theta = \frac{K[L]^n}{1+K[L]^n} \qquad (13)$$

The concentration of unbound ligand, *[L]*, refers to the concentration of ligand that can bind to the binding site. These ligands can only bind to sites that have already been altered by allosteric modulators. The concentration of ligands that are able to bind is directly related to the concentration of allosteric modulators, or reminders. As the concentration of allosteric modulators increases, the concentration of bound ligand increases as well. In the model, the concentration of the unbound ligand is replaced by the concentration of reminders in solution.

The Hill equation calculates θ, which is the fraction of the sites on the receptor protein that are bound by the ligand. In the analogy of mask wearing, this is replaced by the concentration of people in each group who end up wearing a mask, *cM*, because a bound ligand represents an individual that decides to put on a mask. The new equation with the replaced variables is:

$$cM = \frac{K[cR]^n}{1+K[cR]^n} \qquad (14)$$

Chapter 5

Experimental Methodology

5.1 Data Collection Methodology

In order to test the accuracy of the cooperative binding tipping point model, experimental data was collected. This data that was recorded included whether or not individuals wore masks, as well as group size, location, and approximate age group of the acting individuals (child, college student, adult, or elderly). Although this study includes human participants, it did not fall under the requirements for an International Review Board (IRB) application, because no identifying information for the participants was recorded. Confirmation of compliance with the IRB human study policies can be found in Appendix B.

About 600 pieces of data were collected, including individuals who were observed alone and those who were observed in groups. Sites of data collection include various locations on Penn State University's campus, as well as the surrounding areas of State College. Examples of locations include Penn State's Paterno Library, outside on College Avenue in State College, the HUB-Robeson Center, Trader Joe's, Sam's Club, and more. An extensive list of data collection sites can be found in the appendix. Those also involved in data collection include Tim Schmitt and Darrell Velegol.

5.2 Parameter Matrix

The four parameters extracted from the experimental data along with justification for impact on the model are as follows:

1. **Level of trust between individuals**. This factor was noted as the type of relationship between individuals. The types of relationships were broken down into strangers, acquaintances, friends, and family. A larger value for the trust parameter indicates a lower level of trust.
2. **The number of external reminders.** External reminders include signs or posters telling individuals to wear masks, verbal reminders from store or restaurant employees, requirements by law or state ordinances, as well as enforcement by police or other officials. This category is additive, meaning the number of external reminders aggregates and that value is used in the final calculation. More external reminders result in a higher parameter value.
3. **Indoor vs outdoor spaces**. This factor greatly affects a person's decision to wear a mask, especially after CDC guidelines stated that the SARS-CoV-2 virus is more easily spread indoors[15]. This category includes small spaces, such as small rooms or shops, medium spaces, such as a restaurant or bigger store, and large spaces, such as warehouses. A smaller space is given a larger parameter value, since someone in this type of space is likely more inclined to put on a mask.
4. **General health of each individual.** Because no identifying information about the study participants was recorded, this parameter was roughly estimated based on age and any outwardly appearing signs of health such as weight and observed physical aids. Those

with greater health risks are likely more inclined to wear a mask for self-protection, so the value for this parameter increased as health risk increased.

These four parameters were used in the calculation for the concentration of reminders, or *cR.* A higher parameter value indicates a stronger reminder to wear a mask. Parameter values were assigned by asking individuals to rank each of the following scenarios from 0 to 10 for how likely they were to put on a mask, with 0 being not at all likely and 10 being extremely likely. The following scenarios were presented[16]:

1. You see a sign or poster reminding you to wear a mask.
2. Somebody (e.g. an employee) tells you to wear a mask.
3. You are aware that masks are required at your location (either by the government or the store/location).
4. You are aware that mask wearing is being actively enforced at your location (e.g. fines).
5. You are in a large, warehouse-like space (e.g. Costco).
6. You are in a medium sized space (e.g. a restaurant or store).
7. You are in a small space (e.g. a small shop).
8. You are around strangers.
9. You are around people you know, but that you are not close friends with.
10. You are around friends.
11. You are around family.
12. You are around someone who is young (<30 years old).
13. You are around someone who is middle-aged (30-60 years old).
14. You are around someone who is elderly (>60 years old).

15. You are around a seemingly healthy person (healthy weight, no visible disabilities or aids).
16. You are around someone of an unhealthy weight (underweight or overweight).
17. You are around someone with a visible aid or disability (e.g. wheelchair, oxygen tank)

Scenarios 1 through 4 are a subcategory of the *external reminders* parameter, scenarios 5 to 7 address the *indoors/outdoors* parameters, scenarios 8 to 11 address the *trust* parameter, and scenarios 12 to 17 cover the *health* parameter. Preliminary data for the parameter values were taken from members of the Econochemistry lab. A further advancement of this matrix would include obtaining IRB permissions for human subject research to survey a larger population.

These initial data points were used to calculate the mean and standard deviation for each subcategory. Once these were calculated, a parameter matrix was constructed to obtain random values for each subcategory that fall within the mean and standard deviation for each. An example of one iteration is shown below.

RAND(AVG+STDEV)				
Reminders			**Trusted**	
Signs/Posters	0.7800501256		Strangers	0.5794947159
Verbal Reminders	0.9267145038		Acquaintance	0.5712750804
Requirement	0.8775574605		Friends	0.5063623019
Enforcement	0.7737982348		Family	0.7549097443
(Additive)				
Indoor/Outdoor			**Health**	
Outdoor	0		**Age**	
Indoor			Young	0.4505350507
Large space (warehouse)	0.7396716362		Middle-aged	0.6723994902
Medium space (restaurant)	0.8686874888		Elderly	0.7955230592
Small space (room/shop)	0.939511887		**Weight**	
			Healthy weight	0.4977360474
			overweight	0.2609945639
			Observed aids	
			none	0.4297984923
			one or more	0.6781286717

Figure 12. Parameter Matrix

The parameter matrix was used to test the stability of the model by addressing variations in the strengths of the parameters. The model was run several times, and each time a new set of parameter values were updated within the model. This is a place for improvement in future iterations of the proposed cooperative binding model. Additional data points can be collected to solidify the parameters and reduce the standard deviation, and ultimately reduce any fluctuations in the model. By collecting the appropriate data from people in different populations and communities, this model can be applied to more populations than just State College.

Chapter 6

Results and Discussion

6.1 Data Organization

The first step in the analysis of the collected data was to calculate the concentration of people in each observed group wearing masks, *cM*, and not wearing masks, *cN*. Those wearing masks incorrectly, such as under their nose, were counted in the calculation for *cM*, since these individuals had the intention of wearing a mask.

The second step involved the calculation of the concentration of each of the four parameters for each data point collected. This was found through the parameter matrix. The value for trust was found by defining the individuals as friends, family, acquaintances, or strangers, and then assigning the value from the parameter matrix for the corresponding subcategory. The external reminders parameter was additive, which meant adding the values from the parameter matrix for each additional reminder. The external reminders that were considered were signs/posters, verbal reminders, required but not actively enforced, and required and actively enforced. The health concentration was found by taking an average of the relative health levels of those in each group. Health levels were determined by age and any observed visual aids. Since this study was completely anonymous and no identifiable information was recorded, this category was intentionally vague to comply with IRB regulations. A further progression of this study could include more accurate health information. Lastly, the value for the indoor/outdoor parameter was found from the parameter matrix and observing where each data point was collected.

Next, the concentration of total reminders, *cR,* was calculated. This value was calculated using the group contribution method. This method is used in chemistry to predict thermodynamic properties by using the common properties of atoms or groups of atoms in molecules. The total reminder calculation includes all four parameters described in section 5.2. The following equation was used, where [T] is the concentration/parameter value for trust, [E] is external reminders, [IO] is indoors vs outdoors, [H] is health, *M* is the number of people in each group wearing masks, and *W* is the number of people in each group not wearing masks.

$$cR = \frac{1}{c_0}\left(\frac{M-1}{N} * [T] - \frac{W-1}{N} * [T] + [E] + [IO] + [H]\right) \qquad (15)$$

The trust parameter is scaled by the number of surrounding individuals wearing a mask, *M-1,* which positively encourages someone to put on a mask, as well as the number of surrounding individuals not wearing a mask, *W-1,* which negatively impacts someone's decision to put on a mask.

Once the concentration of total reminders, *cR,* was calculated for each data point, the model was applied to predict *cM* for each calculated *cR*. Data points where N<2 were excluded from the calculations because the cooperative binding model hypothesizes how people will behave in larger groups. Then, *cM predict* was calculated:

$$cM\ predict = \frac{KcR^n}{1+KcR^n} \qquad (16)$$

6.2 Data Evaluation

To evaluate the data, the experimental cM, which was found by dividing the number of individuals in each group wearing masks divided by the total number of people in each group, was compared to *cM predict*, as calculated by the model. The goal was to determine if the model's predictions were close in value to the experimental data, and to fit the parameters *K* and *n* to reduce the error as much as possible. The following figure shows an example of five data entries and the corresponding calculations by the model. The first four green columns are the raw data of what was observed, the next four blue columns are the calculations of the individual parameters based on the parameter matrix, and the remaining white columns are the application of the model and error calculation.

N	n mask	n no mask	n wrong	Trust	Ext Reminders	Health	Indoor/outdoor		cM	cN	cR	cM predict	err
16	14	2	0	0.264	1.000	0.600	0.400		0.875	0.125	2.168	1.000	0.125
12	3	9	0	1.087	0.000	0.600	0.400		0.250	0.750	1.239	0.965	0.715
7	7	0	0	0.264	0.000	0.600	0.578		1.000	0.000	1.510	0.998	0.002
12	9	3	0	0.264	2.228	0.600	0.928		0.750	0.250	3.809	1.000	0.250
15	0	15	0	1.087	0.000	0.616	0.928		0.000	1.000	1.553	0.999	0.999

Figure 13. Example of 5 data entries and application of the model

The error was determined by finding the difference between *cM experimental* and *cM predict* for each data point, and then finding a cumulative error by adding each individual error together. This would allow for parameters *K* and *n* to be fit to the data by looking at one overall error rather than hundreds of individual errors.

Extraneous data points were excluded and not counted towards the overall error. This was due to the fact that several data points were skewed due to individual circumstances or exceptions to some mask-wearing rules. These points were manually screened. For example, someone eating would result in an extremely large error. All reminders may lead to the person

putting on their mask, but they don't because they are eating and cannot wear the mask. Otherwise they likely would, and this model doesn't account for this type of circumstance. This should be considered in the refinement of this model.

N	n mask	n no mask	n wrong	Trust	Ext Reminders	Health	Indoor/outdoor		cM	cN	cR	cM predict	err
3		3		1.087	1.419	0.616	1.292		0.000	1.000	3.022	1.000	1.000

Figure 14. Example of large error within the model

In this example line of data, according to the high concentration of reminders, *cR*, the model predicts that the concentration of people in this group that will wear masks is 1, which is that everyone will wear a mask. However, as seen by the high error of 0.9999, the model was completely wrong and this group of people were not wearing masks at all. This is because the people in this group were actively eating, and therefore could not put on their masks. Even though there was a high level of reminders, the exception of eating completely outweighed anything that the model could have predicted, and scenarios like this were not accounted for in this model. If these errors were completely removed, the accuracy of this model would increase significantly, however they were included in the error analysis to note the shortcomings of the model.

To determine the accuracy of the model, an error threshold of 0.2 was applied, meaning that any time the model predicted the concentration of masks, *cM predict*, and was within 0.2 of the experimental *cM*, that prediction was considered to be correct. On average, the model was correct 74.68 ± 0.48% of the time with a 90% confidence interval.

The optimal value for *K* was found to be about 1.11, and the optimal value for *n* was 15. These parameters were optimized manually. The tipping point occurs when the denominator of equation 16 is equal to 2, otherwise written as:

$$cR_{tip} = \exp\left[\frac{-\ln(k)}{n}\right] \qquad (17)$$

The tipping point was found to occur when cR=0.993. Contextually, this means that when the concentration of reminders reaches 0.993 (for this population), the concentration of people who decide to put on their masks increases dramatically.

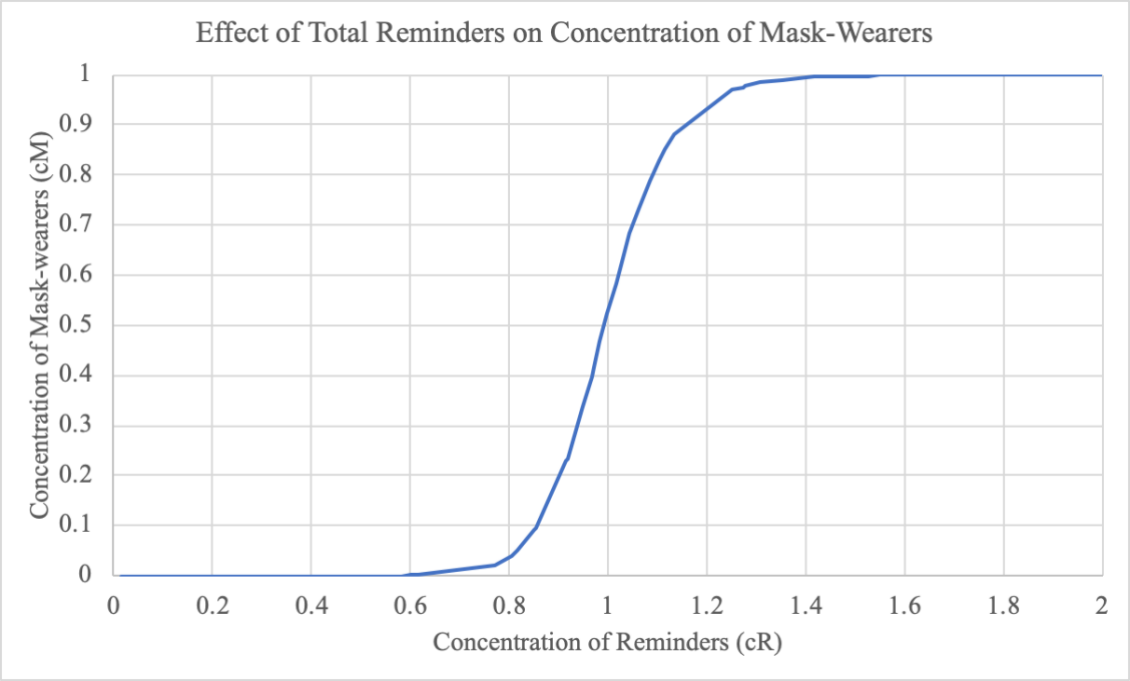


Figure 15. Effect of total reminders on concentration of mask-wearers

The graph shows that a concentration of reminders from 0 to about 0.8 results in a concentration of mask-wearers of 0. This means that this low of a concentration does not have a large enough effect on the population to cause them to put on their mask. Instead of the number of people wearing a mask increasing linearly with increasing concentration of reminders, there is a sigmoidal relationship, as seen with cooperative binding. After the tipping point of 0.993, the concentration of mask wearers increases dramatically. Once the concentration of reminders reaches 1.3, *cM* is essentially 1, meaning everyone in the group is wearing a mask. The existence of this tipping point suggests that there is a specific number of reminders necessary to significantly persuade a population to change their action.

6.3 Stability of the Model

The stability of the model was tested by inputting random numbers into the parameter matrix. These random numbers were calculated using a generator in excel that would generate a number within the mean and standard deviation for each category of parameter. Each time the spreadsheet was reset, a new *cR* and *cM* value would be calculated for each data point, and ultimately a new total error (sum of the individual errors) would be found. This process was run several times such that a variety of errors was collected to be compared across trials. The results are as follows.

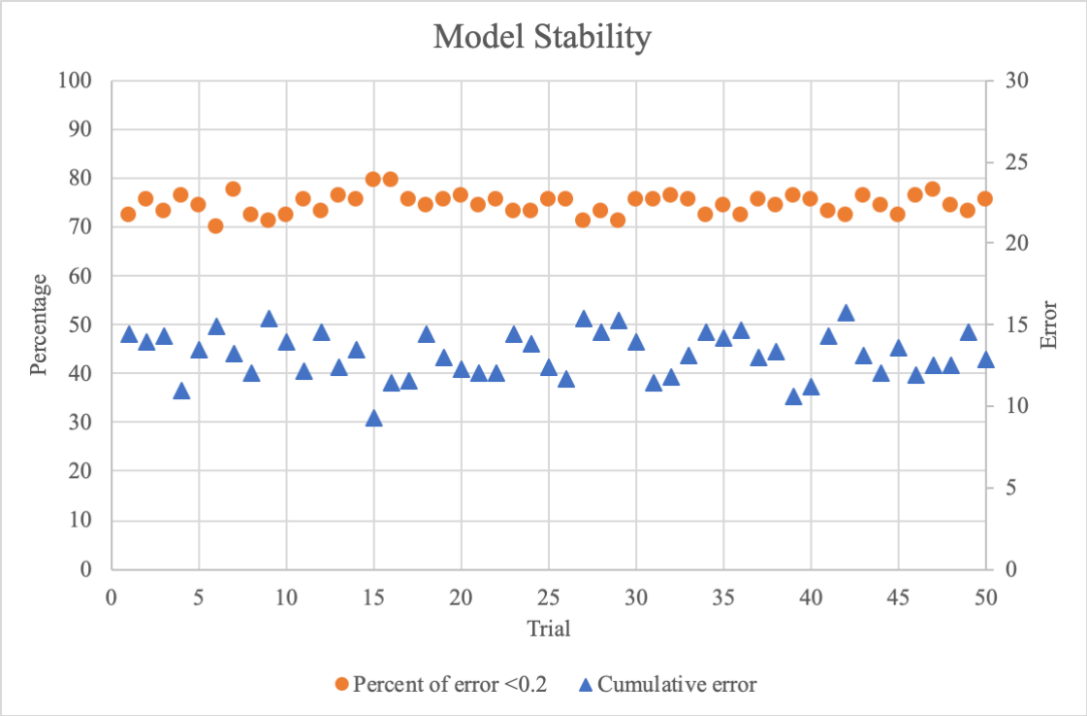


Figure 16. Stability of the model

The model is relatively stable, considering the low sample size of data taken to calculate the parameter matrix. Figure 15 shows minor fluctuations in the percentage of errors less than 0.2, which is how the model was defined as being "correct". The cumulative error saw slightly more fluctuations but overall only ranged from 9.25 to 15.78. The stability will be strengthened as the parameter matrix is further defined. Collecting data with a larger sample size will decrease the standard deviations of the parameter values and therefore reduce how widely the parameter values vary.

6.4 Future Extensions of the Model

This model operated under the assumption that the particles in question (the reminders) were well mixed. This means that the "concentration" of reminders was constant in each scenario that was analyzed. For example, in a restaurant, it was assumed that the concentration of reminders for someone getting up to use the restroom was the same as someone seated at a table, and was the same as someone in the door. In real chemical systems, however, this is not always the case, especially when systems have fewer particles. Take for example, a large box divided into smaller, equal sized boxes. The particles are free to move around the large box, such that on average, the mean number of particles in each smaller box is equal. This is depicted below.

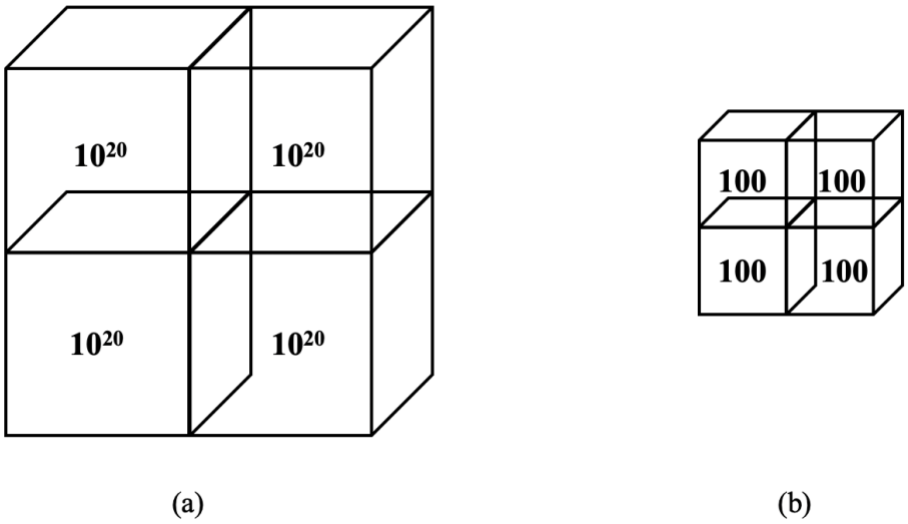


Figure 17. Particles evenly distributed within a box

On average, the compartment shown in Figure 16a has 10^{20} particles in each individual box, and the compartment shown in Figure 16b has 100 particles in each individual box. Since the particles roam freely throughout the entire space, this means that the contents of each smaller

box will vary slightly from the mean at any given time. This variance is found from the following equation:

$$s.d. = \frac{1}{\sqrt{mean}} \qquad (18)$$

The following table compares the relationship between the mean number of particles in each individual box with the corresponding variance.

Table 2. Variances of Particles in a Box

Mean (particles)	Variance
10^{20}	10^{-10}
10^{15}	3.16×10^{-8}
10^{10}	0.00001
10^{5}	0.00316
1000	0.0316
100	0.1
10	0.316
1	1
0.1	3.16

A large mean of 10^{20} has such a small variance that there is essentially a constant number of particles in each box at all times, which can be described as a well-mixed solution. However, as the mean number of particles decreases, the variance increases substantially. This shows that as there are less particles overall, the number of particles in any one section of the box at a given time is not constant. This is analogous to saying that someone standing in the doorway of a restaurant does not experience the same concentration of reminders as someone sitting in the back of the restaurant, since the variance is unknown. A future extension of this model could be to assume the solution is not well-mixed, and to consider how variations in concentration would affect the formation of ligand-receptor complexes in different locations throughout the solution.

Chapter 7

Conclusions

The findings of the model presented in this thesis reveal an alternative method to determine how surroundings and the environment affect the way people make decisions. This model takes mathematical concepts of social tipping points and chemical concepts of micellization and cooperative binding and combines them to provide further insight into how external and internal reminders affect people's decision making. The cooperative binding model was able to accurately predict the outcome of mask-wearing decisions $74.68 \pm 0.48\%$ of the time with a 90% confidence interval, and was found to be most effective when group size, n, was larger than 2.

This model has the potential to be adapted to fit various different populations. The parameter matrix was designed such that any population could be surveyed to determine parameter values, and the concentration of reminders would be calculated accordingly for that population. Further advancements of this research could include surveying populations with varying demographics and comparing the corresponding tipping points to analyze the effect of demographic on tipping point.

In addition to applying this model to different populations, it can also be used to address decisions other than mask wearing. Relating to the SARS-CoV2 pandemic, the next question after whether or not someone wears a mask is whether or not they get vaccinated against the disease. *How does the number of people around you that have been vaccinated change your decision to get vaccinated?* By defining a new set of reminders relating to vaccinations, a new

tipping point can be calculated. The “reminders” in this scenario could include cost, availability, effectiveness, ethical beliefs, and overall health of the patient.

This model is the start of an exciting new field for the combination of social and chemical sciences. The findings of this thesis present a foundational model that can be further developed and adapted to fit new populations and answer new questions.

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(16) Schmitt, T. *Econochemistry Lab member*

Appendix A

AVERAGES				
Reminders			**Trusted**	
Signs/Posters	0.8422222222		Strangers	0.8122222222
Verbal Reminders	0.8755555556		Acquaintance	0.64
Requirement	0.8911111111		Friends	0.3711111111
Enforcement	0.89		Family	0.2922222222
(Additive)				
Indoor/Outdoor			**Health**	
Outdoor	0		**Age**	
Indoor			Young	0.5955555556
Large space (warehouse)	0.7844444444		Middle-aged	0.6844444444
Medium space (restaurant)	0.7955555556		Elderly	0.8511111111
Small space (room/shop)	0.8322222222		**Weight**	
			Healthy weight	0.6111111111
			overweight	0.6933333333
			Observed aids	
			none	0.6
			one or more	0.8355555556

Figure 18. Parameter matrix average values

ST DEV				
Reminders			**Trusted**	
Signs/Posters	0.2880095397		Strangers	0.3167942327
Verbal Reminders	0.2797365283		Acquaintance	0.3366951683
Requirement	0.2372400225		Friends	0.316674641
Enforcement	0.2526226075		Family	0.3394439898
(Additive)				
Indoor/Outdoor			**Health**	
Outdoor	0		**Age**	
Indoor			Young	0.3710890334
Large space (warehouse)	0.3363950299		Middle-aged	0.3617856947
Medium space (restaurant)	0.3059675826		Elderly	0.2920322384
Small space (room/shop)	0.32071574		**Weight**	
			Healthy weight	0.3833003938
			overweight	0.3701351105
			Observed aids	
			none	0.3913844889
			one or more	0.332453384

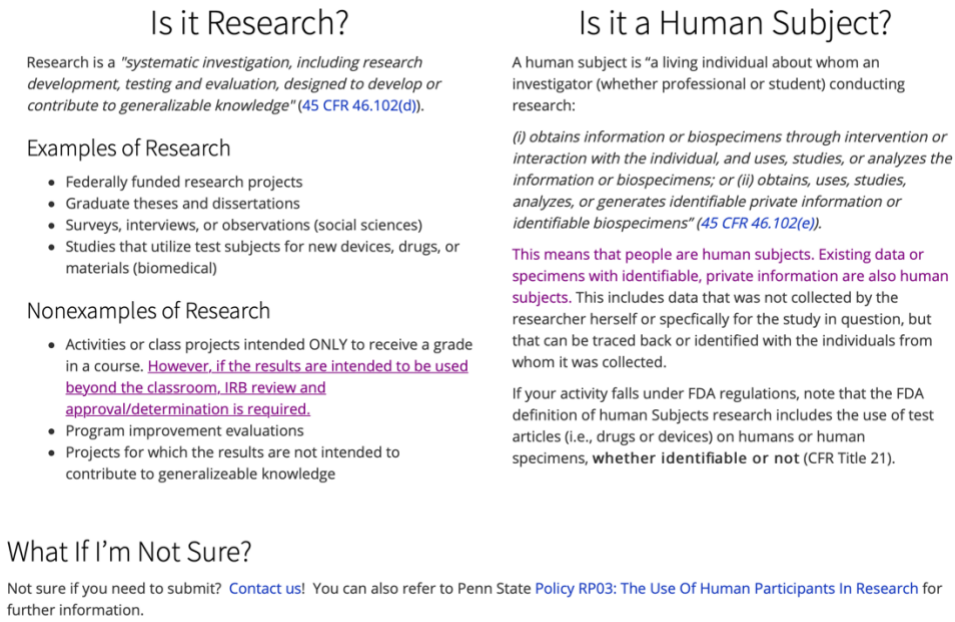
Figure 19. Parameter matrix standard deviation values

List of data collection sites

1. Thomas Building, Penn State University Park Campus
2. Pattee and Paterno Libraries, Penn State University Park Campus
3. HUB-Robeson Center, Penn State University Park Campus
4. Penn State University Park Campus, general
5. Pattee Library Bus Stop, Penn State University Park Campus
6. Trader Joe's Grocery Store, State College PA
7. Bellefonte Park, Bellefonte PA
8. Big Spring, Bellefonte PA
9. Rothrock Coffee, State College PA
10. Wegmans Grocery Store, State College PA
11. College Avenue, Downtown State College
12. Allen Street, Downtown State College
13. Sam's Club, State College PA

Appendix B

IRB Requirements and Exemption



Is it Research?

Research is a *"systematic investigation, including research development, testing and evaluation, designed to develop or contribute to generalizable knowledge"* (45 CFR 46.102(d)).

Examples of Research

- Federally funded research projects
- Graduate theses and dissertations
- Surveys, interviews, or observations (social sciences)
- Studies that utilize test subjects for new devices, drugs, or materials (biomedical)

Nonexamples of Research

- Activities or class projects intended ONLY to receive a grade in a course. However, if the results are intended to be used beyond the classroom, IRB review and approval/determination is required.
- Program improvement evaluations
- Projects for which the results are not intended to contribute to generalizeable knowledge

Is it a Human Subject?

A human subject is "a living individual about whom an investigator (whether professional or student) conducting research:

(i) obtains information or biospecimens through intervention or interaction with the individual, and uses, studies, or analyzes the information or biospecimens; or (ii) obtains, uses, studies, analyzes, or generates identifiable private information or identifiable biospecimens" (45 CFR 46.102(e)).

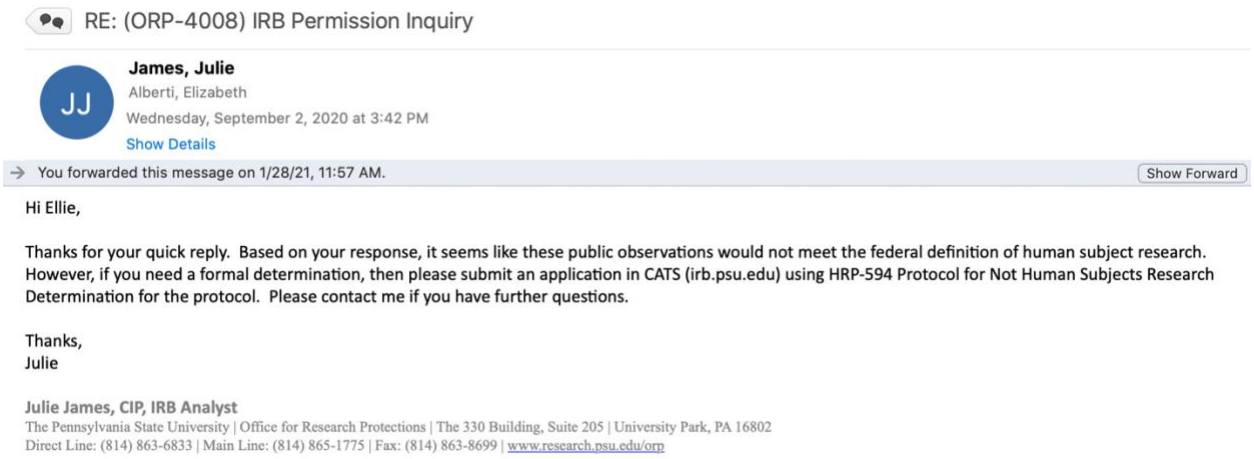
This means that people are human subjects. Existing data or specimens with identifiable, private information are also human subjects. This includes data that was not collected by the researcher herself or specfically for the study in question, but that can be traced back or identified with the individuals from whom it was collected.

If your activity falls under FDA regulations, note that the FDA definition of human Subjects research includes the use of test articles (i.e., drugs or devices) on humans or human specimens, **whether identifiable or not** (CFR Title 21).

What If I'm Not Sure?

Not sure if you need to submit? Contact us! You can also refer to Penn State Policy RP03: The Use Of Human Participants In Research for further information.

Figure 20. Attributes of human subject research that would require an IRB



RE: (ORP-4008) IRB Permission Inquiry

JJ

James, Julie
Alberti, Elizabeth
Wednesday, September 2, 2020 at 3:42 PM
Show Details

You forwarded this message on 1/28/21, 11:57 AM. Show Forward

Hi Ellie,

Thanks for your quick reply. Based on your response, it seems like these public observations would not meet the federal definition of human subject research. However, if you need a formal determination, then please submit an application in CATS (irb.psu.edu) using HRP-594 Protocol for Not Human Subjects Research Determination for the protocol. Please contact me if you have further questions.

Thanks,
Julie

Julie James, CIP, IRB Analyst
The Pennsylvania State University | Office for Research Protections | The 330 Building, Suite 205 | University Park, PA 16802
Direct Line: (814) 863-6833 | Main Line: (814) 865-1775 | Fax: (814) 863-8699 | www.research.psu.edu/orp

Figure 21. Communication with Review Board to show exemption

ACADEMIC VITA

ELLIE ALBERTI

EDUCATION

The Pennsylvania State University | Schreyer Honors College — **University Park, PA**
College of Engineering | Bachelor of Science in Chemical Engineering — *Class of 2021*
Certificate in Entrepreneurship and Innovation

RELEVANT EXPERIENCE

Merck & Co., Inc. — **Upper Gwynedd, PA**
Data Analytics Intern | Global Medical and Scientific Affairs — *May 2020 – Aug 2020*
- Collected and analyzed YTD expense results and adjusted the August financial forecast to reflect a surge in innovative projects and a reduction in travel due to COVID-19, and organized an $85M budget for the organization
- Designed a dashboard to analyze and display financial data by exploring various software such as QlikSense and Tableau
- Worked independently in a remote environment and connected with mentors by participating in Next Generation Network events

Lockheed Martin — **King of Prussia, PA**
Systems Engineering Intern | Rotary and Mission Systems — *May 2019 – Aug 2019*
- Developed a unique system within Jira, an issue management software, to track and store over 800 hardware items in order to create more effective hardware management and lessen the financial burden when equipment is misplaced or goes missing
- Gained experience with 3D modeling software and additive manufacturing by designing and prototyping an end of the year award for the program and leading a scrum team to implement the Agile Methodology

Humanitarian Engineering and Social Entrepreneurship Program — **University Park, PA | Kisumu, Kenya**
MoraSine Venture | Team Lead — *Jan 2019 – May 2020*
- Collaborated on a team of 5 engineers to provide low-cost mobile complete blood count tests to underserved communities in rural areas of Africa who do not have access to affordable healthcare and diagnostic testing
- Performed on-site preliminary research in Kisumu, Kenya to determine the distribution chain for medical devices, medicines, and tests, to test prototypes on potential customers, and to create relationships to foster a sustainable distribution process

Summer by Design Study Abroad Program — **Singapore**
National University of Singapore | Student — *May 2018 – Jun 2018*
- Acquired global design perspective by completing a 3-week accelerated course in engineering design at the National University of Singapore taught by distinguished faculty from Penn State, Brigham Young University, and the National University of Singapore
- Implemented an innovative system-level solution to solve the problem of lost shopping trolleys in Singapore on a team of 5 students by working with FairPrice Markets to increase customer accountability through a custom membership program

Chemical Game Theory Research Lab — **University Park, PA**
Undergraduate Researcher — *Aug 2019 – Present*
- Investigated the use of chemical engineering concepts to provide a more accurate alternative to traditional game theory and human decision making by implementing Gibb's Law of free energy and the entropy of a system to determine an outcome

LEADERSHIP AND INVOLVEMENT

Alpha Kappa Psi Co-Ed Professional Business Fraternity — **University Park, PA**
New Inductee Educator | Special Events Chair | Recruitment Chair — *Sep 2018 – Present*
- Collaborated with 2 co-chairs to orchestrate and host 4 recruitment events, manage a budget of $850, and conduct interviews to select the newest inductee class from over 150 applicants that will uphold the values and standards of the fraternity
- Mentored 20 newly inducted members by hosting biweekly meetings to inform new members of fraternal standards

Global Engineering Fellowship Program — **University Park, PA**
Fellow | Mentor — *Aug 2018 – Present*
- Advised and mentored students about study abroad opportunities by representing the office Global Engineering Engagement, leading outreach programs, and delivering presentations to groups of 25 or more current students, prospective students, and parents

American Institute of Chemical Engineers (AIChE Penn State) — **University Park, PA**
Professional Development Chair — *Jan 2020 – Present*
- Initiated a new professional development program that included resume, interview, and networking workshops, as well as mentoring sessions, guest speakers, and panelists in order to increase involvement and retainment of members

AWARDS, TECHNICAL SKILLS, AND INTERESTS

- **Awards**: SEDTAPP Design Showcase Winner: Most Affective Design, Penn State Academic Excellence Scholarship Award, President's Freshman Award, Phi Eta Sigma National Honor Society, Next Valley Pitch Competition (Third Place), Dean's List (7/7)
- **Software/Skills**: Working knowledge of SolidWorks, Mathematica, Jira, Confluence, Agile, 3-D Printing, QlikSense
- **Laboratory**: Working knowledge of techniques in column chromatography, distillation, recrystallization, and microbial fuel cells
- **Interests**: *Black Mirror,* Water Polo, Homemade Guacamole, National Parks, Cheese Boards, Long Beach Island, Pottery