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CHEMICAL GAME THEORY: ENTROPY IN STRATEGIC DECISION-MAKING

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ABSTRACT

The purpose of this thesis is to describe a framework for representing and solving strategic decision-making problems. Strategic decision-making is frequently analyzed using game theory, but the classical game theory model has several shortcomings. This thesis proposes an alternative method for solving games, in which players' strategies are treated as reactant molecules and equilibrium decisions are evaluated using Gibbsian thermodynamics. This alternative method, called "Chemical Game Theory," removes some of the key shortcomings of classical game theory by including the chemical concept of entropy in the game solution and incorporating player biases, outside enforcer agents, and cardinal payoff magnitudes. This thesis will quantify the relative effects of entropy, perspective, and pre-bias in final equilibrium decisions and discuss how players can adjust their strategies to alter the total welfare and fairness of the outcomes.

TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

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Chapter 1

Introduction

The objective of this thesis is to provide a new way to represent and solve strategic game theory problems[1]. Strategic decisions are those in which players can choose from among two or more possibilities, and the outcome depends upon the collective choices from all players. Strategic decisions are often represented using game theory (here called "classical game theory"), which mathematically models conflict and cooperation between rational individuals.[2] In classical game theory, each player considers the decision-making strategy of their opponents to decide which choice will benefit them most.

Chemical game theory is an alternative representation of strategic decisions, which models these decisions differently and produces different results. Unlike classical game theory, which is a normative theory that addresses what *rational* players *should* do, chemical game theory is a descriptive theory that attempts to predict what *real* players *will* do. It integrates concepts from chemistry and chemical engineering to model strategic decisions via a series of decision reactions, with each player's choices represented as metaphorical molecules.[3]

The thesis will introduce classical game theory, focusing particularly on the Prisoner's Dilemma game, and illustrate the shortcomings of the classical game theory model and relevant literature to address these shortcomings. Then, chemical game theory (CGT) will be introduced as

[1] Parts of this thesis are adapted from Velegol, D., Suhey, P, Connolly, J., Morrissey, N. Cook, L. "Chemical Game Theory," submitted for publication in Industrial and Engineering Chemistry Research, Dec 2017.
[2] Meyerson, R. B. *Game Theory: Analysis of Conflict*, Harvard University Press, 1997
[3] Velegol, Darrell. *Physics of Community Course Notes for Fall 2015.*

an alternative to classical game theory. This thesis will detail the CGT framework, solution methods, and outcomes. It will then analyze the relative effects of payoffs, pre-bias, perspectives, and entropic choices in the decision-making process. Finally, this thesis will analyze how these factors can help determine the best strategy for each player and impact the fairness and total welfare of equilibrium decisions.

Chapter 2

Classical Game Theory

2.1 Representation and Solutions

Classical game theory was developed by John von Neumann and Oskar Morgenstern in their seminal work, *Theory of Games and Economic Behavior*[4], which described the mathematical models upon which modern game theory is based. This later led to the development of the Prisoner's Dilemma game[5], which today is the most well-studied classical game. This thesis will focus on the Prisoner's Dilemma (PD) game, although the methods and solutions of CGT can be applied to other games, including Battle of the Sexes, the Chicken Game, and Tragedy of the Commons[6].

The PD game unfolds as follows. Two players, A and B, decide to rob a bank, but are apprehended immediately before the act. Players A and B are taken to the police station and placed in two different rooms, without the ability to communicate. The district attorney, player D, tells each of them that they have two options: 1) They can remain *quiet*, not revealing that their partner intended to commit the crime. In classical game theory, this strategy is called "cooperating." 2) They can *tell* the district attorney that their partner intended to commit the crime. In classical game theory, this is called "defecting."

[4] Von Neumann, J.; Morgenstern, O. *Theory of Games and Economic Behavior*. Princeton: Princeton University Press, 2007.
[5] The PD game was originally framed in 1950 by Merrill Flood and Melvin Dresher working at RAND Corporation. Albert Tucker formalized the game and named it "prisoner's dilemma." This history is described in: Poundstone, William. "Prisoner's Dilemma." Anchor Books, New York 1992.
[6] Gintis, H. "Game Theory Evolving." Princeton University Press, 2000.

Each of these decisions has an associated payoff, and the final outcome depends on the decisions of both players. If both players A and B remain *quiet* (i.e. do not implicate their partner), they will each only receive one year in prison on a misdemeanor charge. If both players A and B *tell* (i.e. implicate their partner), they both will receive two years in prison for attempted burglary. However, if player A tells on her partner and player B remains quiet, player A will serve no time, and player B will serve three years. This also occurs vice-versa, if B tells and A is quiet.

Classical game theory often represents scenarios like the PD game in normal form, also known as a payoff matrix, shown in Table 1. Normal form includes a number of aspects: 1) Players. This game has two players, A and B. 2) Strategies. Here, Player A's two strategies (quiet and tell) are shown in the left column. Player B's two strategies (quiet and tell) are shown in the top row. 3) Payoffs. These are represented within each box (ex. a1 = quiet, b1=quiet results in +1, +1: a year in prison for each player). Player A's payoff is listed first in each box, followed by Player B's.

Table 1. Prisoner's Dilemma Game Matrix.
Player A can choose possibility a1 or a2, while B can choose possibility b1 or b2. In each of the four payoff blocks, the value on the left belongs to A, and the value on the right belongs to B. For instance, if A tells and B remains quiet (i.e., a2, b1), then A receives 0 years of prison, while B receives 3.

	b1 = quiet	b2 = tell
a1 = quiet	***+1***, +1	***+3***, 0
a2 = tell	***0***, +3	***+2***, +2

Finding the outcome of the Prisoner's Dilemma game can be done by inspection. This is not always the case, as other common games (such as Battle of the Sexes) require a more detailed calculation. But here, one can solve the PD game by considering each player's options, given another player's strategy. If Player B decides to play quiet, Player A can either remain quiet, and receive one year in prison, or tell, and receive no years in prison. Thus, Player A, a rational player who wants to receive less prison time, should tell. Next, if Player B decides to tell, Player A can either remain quiet, and receive three years in prison, or tell, and receive two years in prison. Again, Player A should tell. Thus, regardless of Player B's strategy, Player A does better if she decides to tell.

Player B faces the same game, so also does best by telling. Thus, a Nash Equilibrium exists at {*tell, tell*}, or {*a2, b2*}, meaning that, if both players are "rational", they will tell on their partner 100% of the time. A Nash equilibrium, developed by mathematician John Nash[7], is a solution where neither player can improve their payoff by playing another strategy. For example, if Player A instead decides to tell only 99% of the time, she has deviated from the Nash Equilibrium, and will receive a worse outcome.

The Nash Equilibrium, {*tell*, *tell*}, is the outcome where both players receive two years in prison. However, there is another outcome where they both would have received only one year in prison: {*quiet*, *quiet*}, and thus would have both been better off. And this is the dilemma: by trying to choose the best decision for themselves individually, they get the worst collectively. The solution is not Pareto optimal[8] (in fact, it is the only one of the three blocks that is not), and players end up with a combined total of jail time that is greater than any of the other three options. The PD game is one of the most well-studied games, and has been used to study choices in climate change[9], fisheries[10], and many other tragedy of the commons scenarios[11].

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[7] Nash, J. Non-cooperative Games. *Annals of Mathematics* **1951**, *54* (2), 286-295.
[8] Pareto, V. *Manual of Political Economy*. London: Macmillan, 1971.
[9] Lange, A.; Vogt, C. Cooperation in international environmental negotiations due to a preference for equity. *J. Public Econ.* **2003**, *87*, 2049-2067.
[10] Ostrum, E. *Governing the Commons: The Evolution of Institutions for Collective Action*. Cambridge: Cambridge University Press, 1990.
[11] Hardin, G. The Tragedy of the Commons. *Science* **1968**, *162*, 1243-1248.

2.2 Shortcomings of Classical Game Theory

There are several problems with the classical solution of game theory problems. This thesis will list four. First is 1) The 100% problem. The Nash equilibrium of the PD game is {*tell, tell*}, which means that this solution should occur 100% of the time, if players are rational. Yet when people are placed in PD game scenarios, players do not tell 100% of the time, or sometimes even the majority of the time. In fact, in experimental PD games, players usually tell only about half of the time[12]. Classical game theory has not yet been able to offer a conclusive answer on why cooperation is so prevalent in experimental scenarios.

2) The Epsilon (ε) problem. In the original PD game, the 0-1-2-3 PD game, all payoffs differ by a value of 1. If instead, the payoffs differed by only ε = 0.01, the game would look like that in Table 2. Classical game theory says the outcome is still exactly the same as the original PD game: The players should play the strategy {*a2, b2*}, {*tell, tell*}, in 100% of the instances - it is the only rational solution. This is because for the PD game, classical game theory compares only the ordinal values of each payoff, and not their cardinal values. For the game in Table 2, however, one might expect each of the four blocks to be played almost equally.

Table 2. PD Game Illustrating the ε Problem
When pains differ only by ε = 0.01, rather than 1, classical game theory concludes that the Nash equilibrium will still be {*tell, tell*}.

	b1 = quiet	b2 = tell
a1 = quiet	***1.99***, 1,99	***2.01***, 1.98
a2 = tell	***1.98***, 2.01	***2.00***, 2.00

[12] Sally, D. Conversation and Cooperation in Social Dilemmas: A Meta-Analysis of Experiments from 1958 to 1992. *Ration. and Soc.* **1995**, *7*, 58-92.

3) The Rationality problem. Classical game theory assumes that players are “rational”: they always act in a way that maximizes their own utility. However, if instead the PD game were played not between two strangers, but two trusting friends, or a father and daughter, one may expect the outcome to be very different. It is reasonable to expect that relationships and trust between players, the perspective of each player (whether they are selfish, altruistic, or vengeful), and any bias they may have before the decision would alter the outcome, perhaps causing them to choose “quiet” more than 0% of the time. Yet classical game theory struggles to incorporate these factors into the game solution.

4) The Decider problem. Classical game theory incorporates only the decisions of the two players A and B in the PD game. However, the PD game is described with a district attorney that asks players A and B whether they will confess or tell. The district attorney is usually assumed to be neutral, but what if the district attorney harshly interrogated Player A, and not Player B, because he wants Player B to take the fall? Again, the impact of these outside agents is not incorporated in the classical solution.

2.3 Relevant Literature to Address Shortcomings

Before describing Chemical Game Theory, this thesis will address some developments in classical game theory over the past half-decade that have attempted to address some of the shortcomings described above. Many of them address the most common problem: that experimental players do not always choose “rationally” (i.e. tell) 100% of the time. The first work that attempts to address this is Quantal Response Equilibrium (QRE)[13]. QRE postulates that even rational players make "errors" in choosing, meaning they do not always choose the Nash Equilibrium. The probability of making errors is based on payoff magnitudes and is described by a Boltzmann distribution. However, QRE says that if a game is played several times, the average outcome still reverts to that of classical game theory. As will be shown with CGT, the inclusion of entropy will make the average outcome different than that of classical game theory.

Additionally, classical game theory can incorporate the idea of Bounded Rationality,[14] which postulates that due to cognitive limitations, players a) have an incomplete knowledge of the world, and b) have a finite capacity to process the information they do have. Thus, players make decisions that are "good enough" given the information and time that they have. That is, they "satisfice", rather than "optimize". CGT incorporates players' finite processing capabilities by restricting the amount of choices (reactants), rather than including every possible choice, and recognizing that some choices will not be made because they are slow to compute (kinetically unfavorable). However, CGT acknowledges that decisions that deviate from rationality are not errors or non-optimal solutions, but deliberate player choices given the unique biases, history, and perspectives that each player brings to the game.

Chemical Game Theory readily allows for the incorporation of player and payoff attributes that explain these deviations from the classical model of rationality. The following section will detail the CGT representation of games.

[13] McKelvey, Richard; Palfrey, Thomas (1995). "Quantal Response Equilibria for Normal Form Games." *Games Econ Behavior*, **1995**, 10, 6-38.
[14] Simon, H. A.; "Models of Bounded Rationality." MIT Press, 1997

Chapter 3

Chemical Game Theory

3.1 CGT Representation

Unlike classical game theory, a normative approach of what rational players *should* do, chemical game theory seeks to explain what actual players *will* do. CGT incorporates concepts from chemistry and chemical engineering in a rigorous model which is hypothesized to explain and predict human decision-making. CGT is not a generalization of classical game theory; rather, it represents contested decision problems differently than classical game theory, and generates different solutions.

Chemical game theory is concerned with decision reactions: the chemical reactions between the metaphorical chemical molecules representing the players and their choices to form decisions. It can first be described using a molecular view of the decisions that occur in each player's brain. In the Prisoner's Dilemma game, each player has two choices: quiet or tell, represented for player A as a1 and a2, respectively. Player A also has some anticipation of how Player B will respond, quiet or tell, represented as b1 and b2, respectively. The results of CGT depend on molecules a1, a2, b1, and b2 reacting to form decisions in both Player A's and Player B's brains. As shown in Figure 1, molecules a1, a2, b1, and b2 can react with solid molecule A, which represents Player A's personality, and incorporates their experiences, history, and knowledge. The example in Figure 1 shows molecules a2 and b1 reacting with molecule A under the aid of a catalyst to form A21, which is the contribution that A brings to the {*tell*, *quiet*} decision.

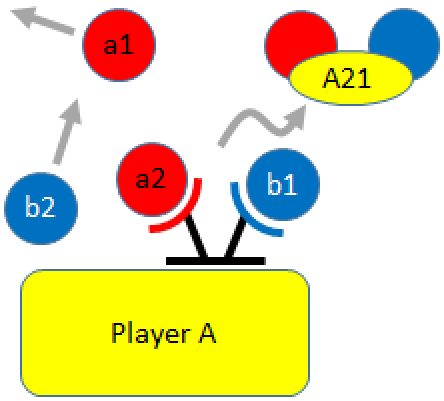

Figure 1. Molecular View of a Decision Reaction.
Choice molecules a2 and b1 react with molecule A to form A21, Player A's contribution to the {*tell, quiet*} decision. The reaction occurs under the aid of a catalyst (the black item with red and blue pockets).

These decision reactions can also be understood at a systems level, detailing the inputs and outputs, shown in Figure 2. The choice inputs a1, a2, b1, and b2 are fed into A's brain, represented as Reactor A. These inputs react with molecule A to form A's four possible decisions in the PD game: A11, A12, A21, and A22. Player A also anticipates what Player B will do when faced with the same inputs, and these reactions occur in reactor B. Here, it is assumed that there is no information asymmetry or deception between the players, although this could be readily included. Thus, each player understands the game completely and accurately, and Player B's diagram will look the same as that for player A.

Here, the Gibbs free energy change ($\Delta g_{\alpha ij}$) values of each reaction, represented in Figure 2 in brackets, are taken directly from the classical PD normal form matrix. These values are nondimensionalized by the thermal energy term *RT*, so that $g_{\alpha ij} = \Delta g_{\alpha ij} / RT$. For example, if A is quiet and B tells (i.e. a1, b2, and A react to form A12), then player A will receive 3 years in prison, and thus the g_{A11}= +3. A higher prison time increases the $g_{\alpha ij}$ value for a reaction, making it less thermodynamically favorable. Though in classical game theory, the values in the matrix represent positive payoffs, this thesis will frame the game in terms of pains (the heat of reaction $\Delta h_{\alpha ij}$), so that a smaller value is more favorable for each player. This thesis will simplify calculations by assuming that $g_{\alpha ij} = h_{\alpha ij}$, where $h_{\alpha ij}$ is also nondimensionalized by $\Delta h_{\alpha ij} / RT$. Thus, the pain for player A associated with the decision A12 is $g_{A11} = h_{A11} = +3$.

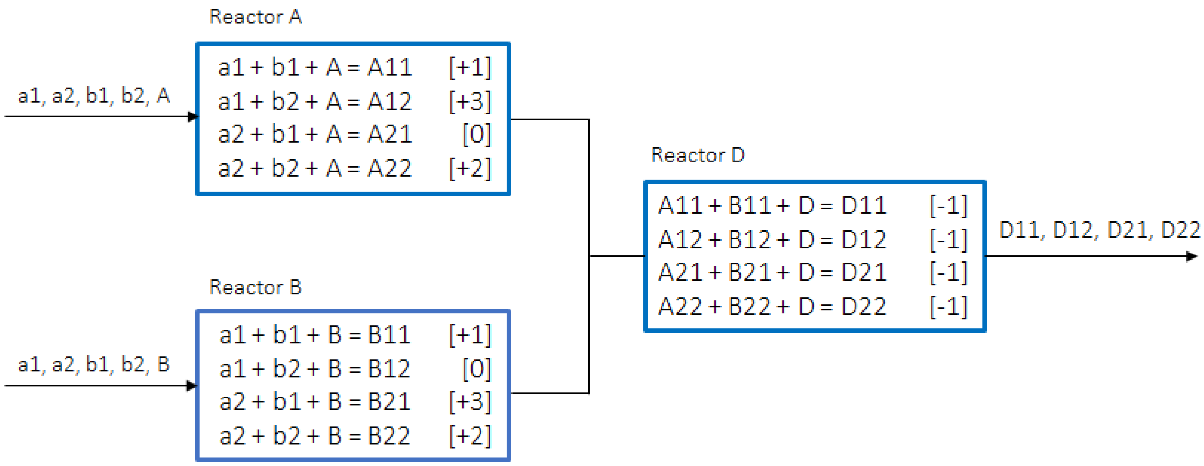

Figure 2. Systems View of Decision Reactions
Block flow diagram for PD game, from A's perspective. It is assumed that B has exactly the same perspective, so that there is no information asymmetry. After species exit each Reactor A, B, and D, a separation step removes unreacted reactants. For example, going into Reactor D, there is no a1, a2, b1, b2, A, or B. Separators are not shown for space considerations.

After reactions occur in Player A and B's brains, the products of each are fed to Reactor D. Before species enter this reactor, a separation step occurs, so that the initial reactants are separated from the mixture and only the products of reactors A and B enter the final reactor D. Player A then must consider how the Decider (Reactor D) will take the inputs from Reactors A and B to make the final decision. In the PD game, Player D is the district attorney, who asks both players whether they will stay quiet or confess. In the game represented in Figure 2, the district attorney is assumed to favor all decisions equally: He feels a pain of $g_{Dij} = -1$ for all decisions.

The products of the D reactor: D11, D12, D21, and D22 represent the concentrations of each of the final four decisions: D11 = {*quiet*, *quiet*}, D12 = {*quiet*, *tell*}, D21 = {*tell, quiet*}, and D22 = {*tell, tell*}. These concentrations are often small, so they are usually normalized with mole fractions ($y_{\alpha ij}$). For example, y_{D12} represents the fraction of the time that Players A and B end up the in {*quiet, tell*} block, where Player A gets 3 years in prison, and Player B gets 0 years. Since evaluating the final concentrations involves solving for the extents of 12 reactions simultaneously, equilibrium decision concentrations are usually solved numerically, using Excel or GAMS. Solutions to chemical games will be detailed in the next section, and the Appendix.

3.2 CGT Solution Methods

The outcomes of each of the twelve reactions shown can be calculated either thermodynamically or kinetically. Using a thermodynamic approach, one can begin with Equation 1:

$$(1) \qquad dG = -SdT + VdP + \sum \mu_i dn_i$$

Where G is the Gibbs free energy, S is the entropy, T is the temperature, P is the pressure, V is the volume, μ_i is the chemical potential of species i, and n_i is the moles of species i. Using the derivation shown in the Appendix, the criteria for equilibrium is:

$$(2) \qquad \Delta g^0 = -RT \ln\left(\frac{p}{p^0}\right) \sum v_i - RT \sum v_i \ln y_i$$

Where R is the ideal gas constant, p^0 is standard pressure, υ_i is the stoichiometric coefficient of each species, and y_i is the mole fraction of species i. All calculations in this thesis assume room temperature and $p/p^0 = 1$, though future work will focus on the effects of temperature and pressure on decision outcomes. The second term on the right-hand side is the entropy of mixing component of chemical reactions, an essential piece of decision reaction equilibrium. The thermodynamic approach then involves for an extent of reaction that satisfies Equation 2. In Excel, this is done with Solver, minimizing the difference between the right-hand side and each of the $g_{\alpha ij}$ values taken from the pain matrix.

Alternatively, this equation is more simply written as an equilibrium constant (K). In CGT, an equilibrium constant can be written for all twelve reactions. For instance, for the reaction that produces A12 (i.e., a1 and b2 reacting to form A's quiet-tell decision), the equilibrium constant is:

(3) $$K_{A21} = \frac{y_{A12}}{y_{a2} y_{b1}} = e^{-g_{A21}}$$

Where g_{A21} is the nondimensionalized molar Gibbs free energy of reaction, given in the payoff matrix as the pain for player A in the a1-b2 block as +3, and $y_{\alpha ij}$ is the mole fraction of each species. The next step is to solve for the 12 mole fractions using a stoichiometric table. The stoichiometric table lists the species, initial concentrations, change in concentrations, end concentrations, and final $y_{\alpha ij}$ mole fractions. Initial concentrations in the CGT model represent the player's pre-biases. In this example, players are assumed to be "unbiased" (i.e. do not favor either decision before the game begins), with all initial reactant concentrations set to $c_{0a1} = c_{0b1} = 0.5$. A table for Player A is shown. Player B's table would look similar, but produce four different decisions (B11, B12, B21, and B22).

Table 3. Stoichiometric Table for Player A.
The stoichiometric table shows the initial, change, and final concentrations, as well as the mole fraction of each species. In this example, player A is unbiased since the amount of a1 and a2 are the same. Additionally, the solid species representing player A does not appear in this table, as solids are often approximated as having a chemical activity of 1. The extents ($\varepsilon_1 – \varepsilon_4$) are written for the four reactions that occur in Reactor A.

species	initial	change	end	y mole fraction
a1	0.50	$-(\varepsilon_1+\varepsilon_2)$	$0.50-(\varepsilon_1+\varepsilon_2)$	$[0.50-(\varepsilon_1+\varepsilon_2)]/\sum$
a2	0.50	$-(\varepsilon_3+\varepsilon_4)$	$0.50-(\varepsilon_3+\varepsilon_4)$	$[0.50-(\varepsilon_3+\varepsilon_4)]/\sum$
b1	0.50	$-(\varepsilon_1+\varepsilon_3)$	$0.50-(\varepsilon_1+\varepsilon_3)$	$[0.50-(\varepsilon_1+\varepsilon_3)]/\sum$
b2	0.50	$-(\varepsilon_2+\varepsilon_4)$	$0.50-(\varepsilon_2+\varepsilon_4)$	$[0.50-(\varepsilon_2+\varepsilon_4)]/\sum$
A11	0	$+\varepsilon_1$	ε_1	$\varepsilon_1/\sum$
A12	0	$+\varepsilon_2$	ε_2	$\varepsilon_2/\sum$
A21	0	$+\varepsilon_3$	ε_3	$\varepsilon_3/\sum$
A22	0	$+\varepsilon_4$	ε_4	$\varepsilon_4/\sum$
total	$\sum_0 = 2.00$	$-(\varepsilon_1+\varepsilon_2+\varepsilon_3+\varepsilon_4)$	$\sum = 2.00-(\varepsilon_1+\varepsilon_2+\varepsilon_3+\varepsilon_4)$	1.00

Reactor D can be similarly represented with a stoichiometric table (Table 4). The reactants for D are the 8 products from Reactors A and B, which each react to create final decisions D11, D12, D21, D22. The mole fractions of each of these four final decisions give the proportion of the time that a particular result, for example D11 = {*quiet, quiet*}, would occur for these players with given pre-biases.

Table 4. Stoichiometric Table for Player D

The Gibbs free energy changes for the four reactions of the Decider are g_{Dij} = -1, unless otherwise specified.

species	initial	change	end	y mole fraction
A11	ε_1	$-\varepsilon_9$	$\varepsilon_1 - \varepsilon_9$	$(\varepsilon_1 - \varepsilon_9) / \sum$
A12	ε_2	$-\varepsilon_{10}$	$\varepsilon_2 - \varepsilon_{10}$	$(\varepsilon_2 - \varepsilon_{10}) / \sum$
A21	ε_3	$-\varepsilon_{11}$	$\varepsilon_3 - \varepsilon_{11}$	$(\varepsilon_3 - \varepsilon_{11}) / \sum$
A22	ε_4	$-\varepsilon_{12}$	$\varepsilon_4 - \varepsilon_{12}$	$(\varepsilon_4 - \varepsilon_{12}) / \sum$
B11	ε_5	$-\varepsilon_9$	$\varepsilon_5 - \varepsilon_9$	$(\varepsilon_5 - \varepsilon_9) / \sum$
B12	ε_6	$-\varepsilon_{10}$	$\varepsilon_6 - \varepsilon_{10}$	$(\varepsilon_6 - \varepsilon_{10}) / \sum$
B21	ε_7	$-\varepsilon_{11}$	$\varepsilon_7 - \varepsilon_{11}$	$(\varepsilon_7 - \varepsilon_{11}) / \sum$
B22	ε_8	$-\varepsilon_{12}$	$\varepsilon_8 - \varepsilon_{12}$	$(\varepsilon_8 - \varepsilon_{12}) / \sum$
D11	0	ε_9	ε_9	$\varepsilon_9 / \sum$
D12	0	ε_{10}	ε_{10}	$\varepsilon_{10} / \sum$
D21	0	ε_{11}	ε_{11}	$\varepsilon_{11} / \sum$
D22	0	ε_{12}	ε_{12}	$\varepsilon_{12} / \sum$
total	$\sum_0$	Δ	$\sum = \sum_0 + \Delta$	1.00

It is now possible to solve for the 12 extents of reaction (ε_i), which will give the final mole fractions from the D reactor, representing the decision outcome. For a PD game with two players, each with two choices, this system can be solved with Excel Solver. For larger systems, Mathematica or GAMS can be used. The next section will detail the results of these calculations.

Chapter 4

Chemical Game Theory Solutions

In classical game theory, the Prisoner's Dilemma game has one Nash Equilibria: both players tell on their opponent and receive 2 years in prison. This is a pure strategy Nash Equilibria, so the result occurs 100% of the time. Using the notation in CGT, this means that the mole fraction y_{D22} = 1.00. In classical game theory, players do not consider information about their opponent, but instead look at their own pains and conclude that, no matter what their partner does, their own pain is minimized by choosing *tell*. However, in CGT, players consider the energetics of their options and include the choice concentrations of their opponent to produce different solutions.

For two unbiased players playing a 0-1-2-3 PD game, the CGT solution, using the methods described in the previous section, is y_{D11} = 0.523, y_{D12} = y_{D21} = 0.183, and y_{D22} = 0.111. That is, the {*quiet, quiet*} decision occurs 52.3% of the time, rather than 0% of the time, and the {*tell, tell*} decision occurs 11.1% of the time, rather than 100% of the time. This result illustrates a few important features of chemical game theory. First, it illustrates the role of "entropic choices." In a chemical reaction, entropy ensures that there is never a 100% extent of reaction. In chemical game theory, entropy ensures that a decision never occurs 100% of the time. Having finite probabilities for both *quiet* and *tell* for this PD game is not due to shortcomings of the player, errors, or irrationality, but rather due to the effect of entropy in the choices.

Another important feature of this CGT solution is that players incorporate information about the game and their opponent to yield an equilibrium decision that is primarily cooperation. The D11 outcome is preferred by unbiased players in CGT, and is played 52.3% of the time. This outcome has the lowest combined total pain (or in the PD game, the least jail time): 1 year for each player, and 2 years in total. All other blocks have a combined total of 3 or 4 years. But unlike classical game theory, which seeks to minimize a player's worst outcome, in CGT players consider their opponents and their choices, and decide to cooperate the majority of the time. There is no "dilemma" in the CGT solution of the PD game, since the actions of each player primarily yield the result that most benefits both themselves and the collective group.

This solution and analysis holds for two unbiased players ($c_{0a1} = c_{0b1} = 0.5$), concerned for only their own pain (consider their own $g_{\alpha ij}$ values), and an unbiased decider (all $g_{Dij} = -1$). It also used the cardinal payoffs in the original PD game (0-1-2-3). However, all of these factors could be changed to analyze the impact that each has on the CGT solution. The rest of Section 4 will detail the results when these parameters are changed.

4.1 Cardinal Payoff Values: The Epsilon Problem

This thesis has discussed how CGT addresses 1) The 100% solution problem, by indicating the probabilities of each of the four outcomes occurring. CGT also addresses 2) The Epsilon (ε) problem, the PD game with pains that differ by only a very small amount, by incorporating the numerical pain of each decision into the thermodynamic calculation via the $g_{\alpha ij}$ values. As ε become small, the calculated pains become closer together (Table 5). The classical solution indicates that {*tell, tell*} will be the only outcome 100% of the time, even if $\varepsilon = 0.01$. CGT shows that decisions do in fact become less differentiated as pain values become closer together, until they are almost all equally likely. When $\varepsilon = 0$, all pains are equal, and thus all decisions occur with equal probabilities. When $\varepsilon = 1$, the solution is that of the 0-1-2-3 PD game detailed in the previous section. This figure reveals the importance of entropic choices, where entropy aims to distribute the outcomes fairly when the pains between different outcomes are not greatly impacted by energetics.

Table 5. PD Game Matrix in Terms of ε
This table is used to construct Figure 3. ε values were changed from 1 (original PD game) to 0 (all pains = 2). At ε = 0.01, pain values are equal those in Table 2, shown prior (i.e. g_{A11} = 1.99, g_{A12} = 2.01, g_{A21} = 1.98, g_{A22} = 2.00).

	b1 = quiet	b2 = tell
a1 = quiet	***2-ε***, 2-ε	***2+ε***, *2-2ε*
a2 = tell	***2-2ε***, *2+ε*	***2***, 2

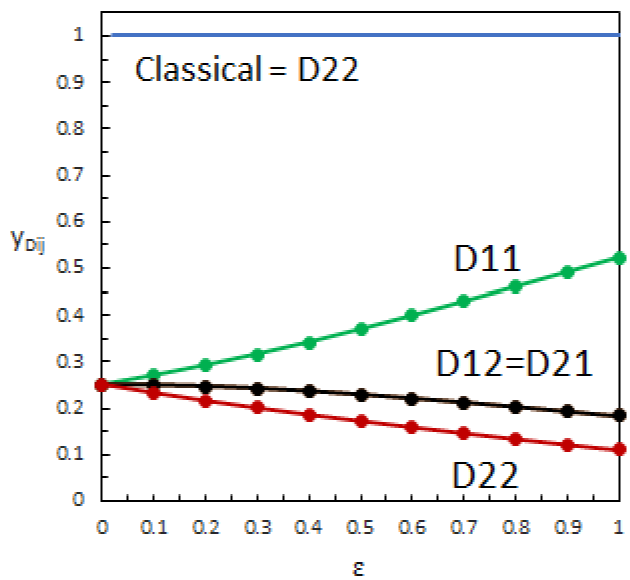

Figure 3. Classical and CGT Solutions for Changing Epsilons
Dij values for two unbiased players for the game in Table 8. As ε values decrease, the final decisions become equally likely. Classical game theory predicts that in the range of $0 < \varepsilon < 1$, the overall solution does not change, and the Nash Equilibrium remains at 100% D22 (i.e.,= tell, tell). No classical NE is given for when ε=0 (all pains the same). In CGT, Dij values change as the relative pains change, as expected from human behavior.

4.2 The Role of the Decider

Chemical game theory, unlike classical, can incorporate outside agents who may impact the game, in addition to the two players themselves. This addresses 3) The Decider Problem, discussed in Section 2.2. In the PD game, Player D is the district attorney, who asks both players whether they will stay quiet or confess. In some situations, Player D might actually be Player A or

Player B, an electronic or regulatory mechanism, or something else that takes the inputs from A and B to make a decision. In the solution method shown earlier, the g_{Dij} values for the Decider are assumed to be -1 for all cases, so that the decider equally favors any decision being made.

However, the decider could instead be biased towards a favorable decision for players (g_{D11} is more negative), show a bias against A or B (g_{D12} or g_{D21} are more negative, respectively), or want them both to take the fall (g_{D22} is more negative). The figure below illustrates the result when g_{D22} is changed and all others are held constant. The decision D11 {*quiet*, *quiet*} still dominates when the decider is neutral or biased against the D22 {*tell*, *tell*} decision, but a decider that very strongly favors D22, and would for example harshly interrogate the players until they confess, can cause the D22 decision to dominate when $g_{D22} < -4$.

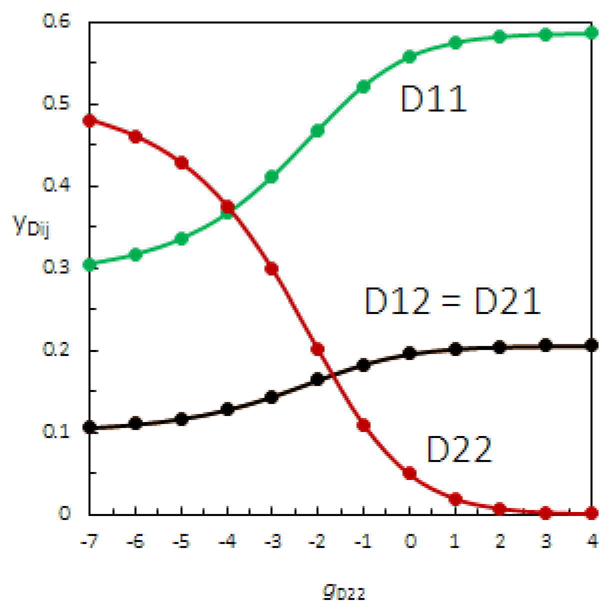

Figure 4. Impact of Decider g_{22} Values
When decider pains for {*tell*, *tell*} are changed, while the pains for the other three decisions are held constant, the {tell, tell} decision can either dominate (at low g_{D22} values) or approach 0 frequency (at high g_{D22} values).

4.3 Incorporating Bias

The next two sections of this work address the final shortcoming of classical game theory: 4) The Rationality problem. In classical game theory, rational players are assumed to have no preference for either choice prior to the game. In CGT, each player enters the game with a certain "pre-bias": their ideas about their possible strategies and their view of their potential payoffs. In CGT, pre-bias is represented as initial concentrations of a1, a2, b1, and b2, where $c_{0a1} + c_{0a2} = 1.0$ and $c_{0b1} + c_{0b2} = 1.0$. In the example solution, all initial concentrations were assumed to be equal at 0.5, so the players were unbiased. However, real players may not choose to behave this way. For example, if a player is an economics major and has heard before about the PD game and its Nash Equilibria, perhaps they know before the game is played that they will choose "tell" more often than they will choose "quiet" (larger c_{0a2})[15]. This result has in fact been observed experimentally[16]. Conversely, if a player decides before playing the game that they would prefer to choose "quiet", they would have a larger value of c_{0a1}.

As shown in Figure 6, different pre-biases can result in significantly different equilibrium outcomes. In Figure 6a, the initial concentrations of Players 1 and 2 are equal and varied together, from 0.02 to 0.98. On the left side of plot a, where c_{0a1} and c_{0b1} are small, the primary outcome is D22. This is expected, since players are biased towards *tell*. However, once $c_{0a1} > 0.4$, D11 is the primary outcome. In going from 3b to 3d, there is an increase in the fraction of D11 {*quiet, quiet*} played at the right side of the plots. Thus, while unbiased players prefer D11 52.3% of the time,

---

[15] Laura Cook in her SHC thesis is able to predict quantitatively the pre-biases in a study of economics and non-economics majors playing an experimental PD game.

[16] Frank, R.; Gilovich, T.; Regan, D. "Does Studying Economics Inhibit Cooperation?" *J. Econ. Perspect.* **1993**, *7*, 159-171

players biased towards *quiet* can cause D11 to dominate even greater than 99% of the time. Conversely, players that are initially biased towards *tell* (high c_{0a2} or c_{0b2}) move the decision toward less cooperation (sometimes choosing D11 even less than 1% of the time), indicating that the initial bias of information can dominate final decisions.

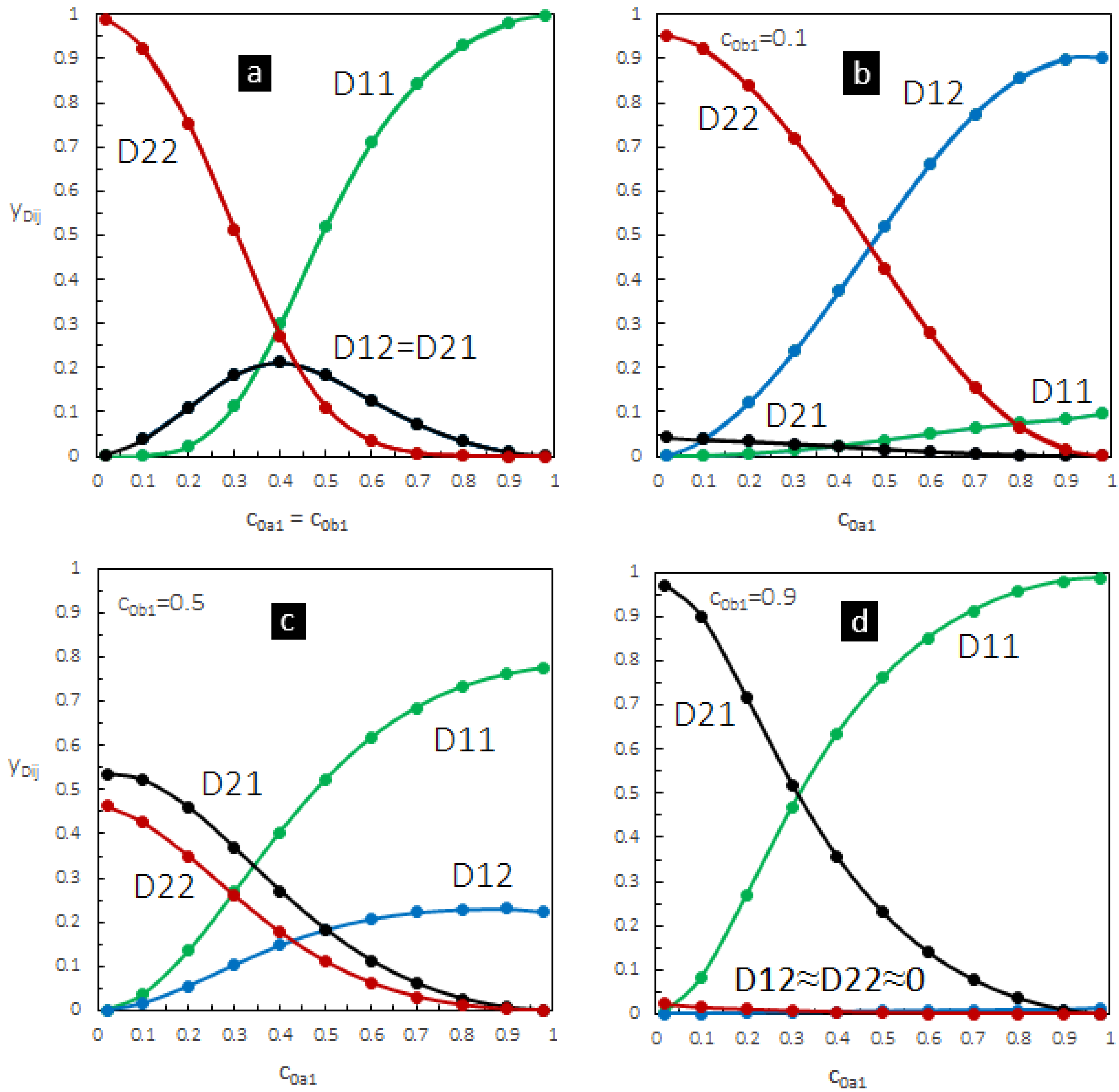

Figure 5a-d. Impact of Pre-Bias on Equilibrium Decisions
Final outcomes y_{Dij} (mole fractions) for players in a PD 0-1-2-3 game. a) $c_{0a1} = c_{b01}$. b) $c_{b01} = 0.1$ (B is biased to stay quiet). c) $c_{b01} = 0.5$ (un-biased). d) $c_{b01} = 0.9$ (B is biased to tell). At the left side of plot (a), where c_{0a1} and c_{b01} are small, the primary outcome is D22 as expected. Once $c_{0a1} = c_{b01} > 0.4$, D11 is the primary outcome. In going from (b) to (d), there is an increase of D11 (quiet-quiet) at the right side of the plots.

The three factors analyzed thus far that influence how each player plays are: 1) The initial choice concentrations, which represent pre-bias. Without significant initial concentrations of a species, it is not possible for certain decisions to dominate. 2) Pains, or $g_{\alpha ij}$ values, which bias the results towards one choice or another. As the difference between pain values increases, the frequency with which decisions are chosen moves further apart. 3) Entropy, which aims to distribute the outcomes fairly, and ensures that no solution will occur 100% of the time, no matter how extreme the pre-bias or pain values.

4.4 Incorporating Perspective

The last aspect of players that the CGT model can incorporate is perspective. Perspective allows for the inclusion of a player's attitude toward others, not as permanent personality traits, but as moods that can depend on who the player's opponent is. For example, a father playing against his daughter in a Prisoner's Dilemma game might be more willing to sacrifice himself than he would be for a casual acquaintance or an enemy. Thus, perspective differs from a player's pre-bias because it changes the way players view the pains in a game - a father may actually receive more pain if his daughter goes to jail than he would receive if he goes to jail.

Perspective is modeled by altering the $g_{\alpha ij}$ values that are represented in the pain matrix. In classical game theory, players are always assumed to be *selfish*: They seek solely to minimize their own pain, without regard to their opponent's outcome. However, in the above example, a father may care nothing for his own pain, and care only about minimizing his daughter's pain. Thus, his $g_{\alpha ij}$ value would be equal to that of his daughter's. This perspective is known as *altruistic.*

The impact of perspective can be modeled by calculating a new $g_{\alpha ij}$ value for a player for each of the four decisions. For each decision, the new $g_{\alpha ij}$ value is the sum of a player's own pain (here defined as $g^0_{\alpha ij}$), times the fraction each person cares about their own pains (C_1), and their opponent's pain, $g^0_{\beta ij}$, times the fraction they care about their opponent's pains (C_2)[17]. This is represented with Equation 4:

(4) $$g_{\alpha ij} = C_1 g^0_{\alpha ij} + C_2 g^0_{\beta ij}$$

Where the sum of the absolute values of C_1 and C_2 is equal to 1. Table 6 shows examples of common perspectives that players can adopt in CGT. For example, if two trusting friends played a PD game, they may both choose to play *overall*: They care equally about minimizing their own pain and their opponent's pain, and thus their $g_{\alpha ij}$ value is the average of the two pains in each block. The new pain matrix for the overall case is shown in Table 7, and the remainder of the games are shown in the Appendix.

Table 6. C1 and C2 Values for Varying Perspectives
These values can range from -1 to 1 for each player, and determine that amount that players care about their opponent's outcome (either favorably or unfavorably).

Perspective	**C1**	**C2**
Selfish	1	0
Altruistic	0	1
Overall	0.5	0.5
Rival	0.5	-0.5
Vengeful	0	-1

Table 7. Pain Matrix if Player B is Overall
Player A has the same perspective as in the original game (selfish), but now player B considers his outcomes by incorporating both his and his partner's pains.

	b1 = quiet	b2 = tell
a1 = quiet	***1***, 1	***3***, *1.5*
a2 = tell	***0***, *1.5*	**2**, 2

[17] John Connolly, *Altruistic to Vengeful Perspectives in Gibbsian Game Theory,* Spring 2016 SHC Thesis.

Two final perspectives considered in this thesis are rival and vengeful, shown in Table 6. This could occur if the players in the PD game are enemies, or even acquaintances who primarily want their opponent to take the fall. Rivalrous opponents care equally about *minimizing* their own pain and *maximizing* their opponent's pain, and thus multiply their own pain ($g_{\alpha ij}$) by 0.5, and their opponent's pain ($g_{\beta ij}$) by -0.5. Thus, higher pains for an opponent are more favorable for a rivalrous player. Vengeful opponents care nothing for themselves, and only for maximizing their opponent's pain, and thus multiply their opponent's pain by -1.

The effects of varying perspective, like those of varying pre-bias, can be analyzed to determine the impact of perspective on equilibrium decisions. The results of changing perspective are not as extreme as those of changing pre-bias. This is because perspective alters pain values, making a particular decision more or less favorable, while pre-bias can significantly reduce the initial concentration of certain species, resulting in a minimal extent of reaction for particular decisions. In Figure 7, A plays with an unbiased, selfish perspective, as in the initial example. Player B is unbiased but consecutively exhibits perspectives of altruistic, overall, rivalrous, and vengeful in plots a-d.

In Figure 7a, where player A is selfish and player B altruistic, player A does very well, since both players are concerned with minimizing player A's pain. Decision D21 (where player A gets 0 years in prison, and player B gets 3) dominates D11 at pre-bias levels of up to $c_{0a1} < 0.65$, where for two selfish players it only dominated D11 up to $c_{0a1} < 0.35$. Moving from b to d, the D21 fractions decrease on the left side of the plots, as player B considers player A's pain less and then begins to view it negatively. Moreover, as player B takes on a less favorable perspective to player A, it is more likely that both will end up in the D22 = {*tell*, *tell*} block, the classical solution where both players get two years in prison. It is worth noting, however, that if player A plays with a high pre-bias towards quiet (c_{0a1} > 0.65), the D11 = {*quiet*, *quiet*} decision will dominate regardless of player B's perspective.

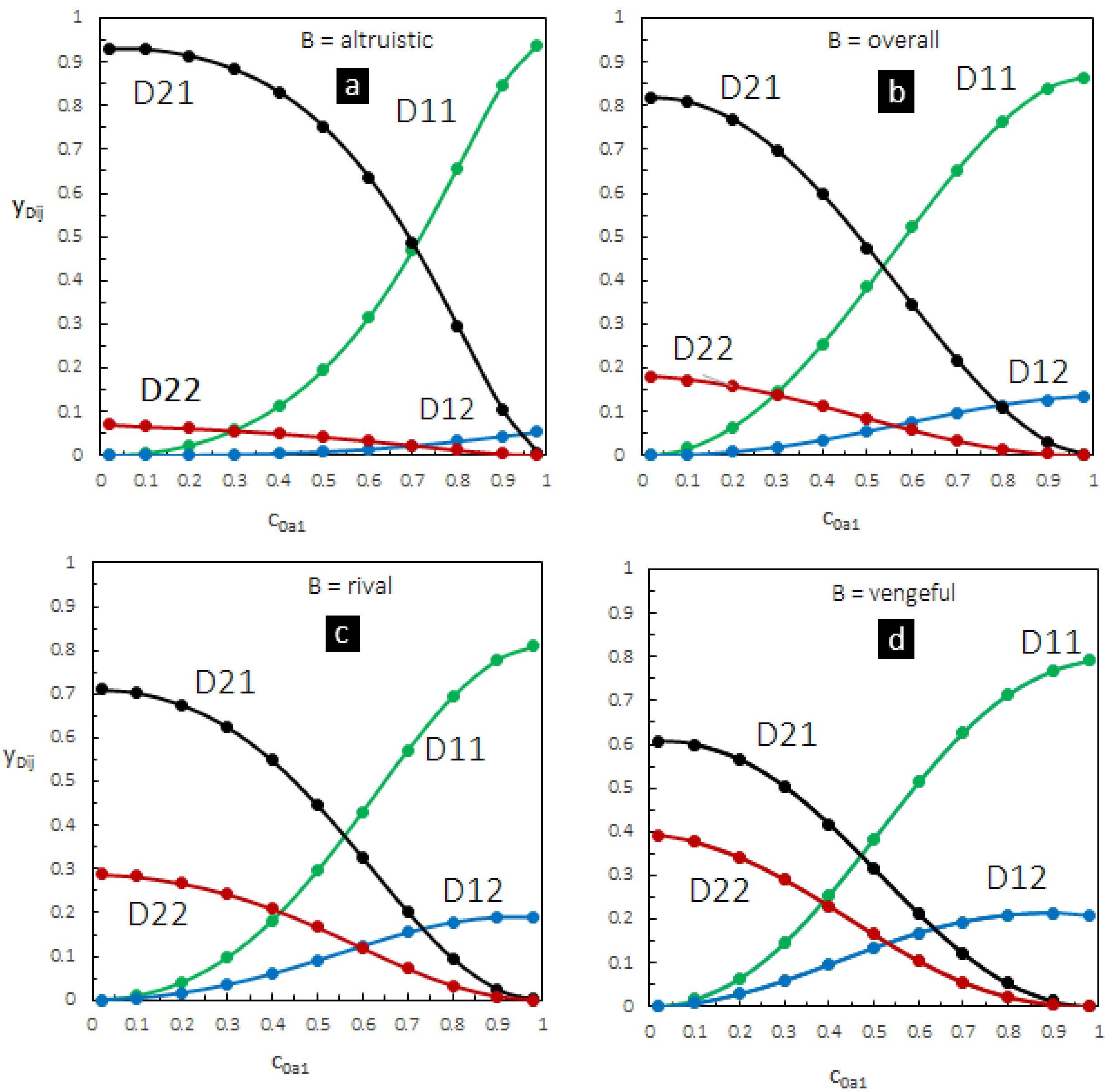

Figure 6a-d. Impact of Perspective on Equilibrium Decisions
Final outcomes y_{Dij} (mole fraction) for players in a PD 0-1-2-3 game, with varying perspective of B. a) Altruistic b) Overall c) Vengeful d) Rival. This illustrates that the consideration of an opponent's pain can cause otherwise less favorable decisions to dominate (here, D21), but also that perspective is not as impactful as pre-bias on altering equilibrium outcomes.

The results of these four sections detail the relative impacts of changing pain magnitudes, decider biases, player pre-bias levels, and player perspectives. The differences between pain magnitudes change how frequently each decision will be played, and how much a particular decision will dominate. Incorporating the role of the decider allows the district attorney to favor one decision over another and influence the final outcome. Pre-bias changes the initial concentrations of choice species a1, a2, b1, and b2. And finally, perspective aims to account for how a player feels about their opponent's outcome by incorporating their opponent's $g_{\alpha ij}$ value.

Studying these game characteristics makes it possible to answer a question posed in the final section of this thesis: "Given my opponent's strategy, including their perspective and pre-bias, how should I play"? With CGT, it is possible to integrate various game and player attributes to produce an answer.

Chapter 5

Analysis of Fairness, Welfare, and Best Responses

The idea of a “best response” is an important concept in classical game theory. In the classical model, finding a best response can be accomplished most simply by determining which strategy results in the highest utility for a player, given a fixed strategy of their opponent. If a player knows their opponent’s *beliefs* (the probability their opponent will play each strategy) then a player can calculate the fraction of the time they should play each of their own available strategies in order to maximize their payoffs. This is known as a Bayesian game[18], where players analyze games with incomplete information, but can incorporate their knowledge of their opponents and their reputations to pick the most rational solution.

However, CGT does not assign a “rational” designation; instead, players can learn in an evolutionary way that some decisions benefit them more than others. Additionally, players can alter not only their strategies, but also their pre-bias and perspective, to result in an equilibrium decision that is more favorable to them. Players can do this by considering their expected pain per decision, or Δh_α values. This is analogous to the concept of expected payoff in classical game theory. A player’s expected payoff is calculated by multiplying a player’s pain for each outcome by the fraction of their decisions in each outcome. In CGT, the role of other players and the Decider is considered, and so Δh_α is calculated by multiplying a player’s pain for each outcome by the concentrations of the final decisions. For the PD game, this is described for players A and B in equations 5 and 6, respectively.

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[18] Harsanyi, J. C.; “Games with Incomplete Information Played by “Bayesian” Players” J. Manag. Sci. **1967**, 159-182.

(5) $$\Delta h_A = \frac{\varepsilon_{D11}h_{A11} + \varepsilon_{D12}h_{A12} + \varepsilon_{D21}h_{A21} + \varepsilon_{D22}h_{A22}}{\varepsilon_{D11} + \varepsilon_{D12} + \varepsilon_{D21} + \varepsilon_{D22}}$$

(6) $$\Delta h_B = \frac{\varepsilon_{D11}h_{B11} + \varepsilon_{D12}h_{B12} + \varepsilon_{D21}h_{B21} + \varepsilon_{D22}h_{B22}}{\varepsilon_{D11} + \varepsilon_{D12} + \varepsilon_{D21} + \varepsilon_{D22}}$$

Where $h_{\alpha ij}$ is taken from the pain matrix (equal to $g_{\alpha ij}$) and ε_{Dij} is the extent of each of the four decisions in the D reactor. Since there is a 1:1 stoichiometric ratio of the reactants and products, the extents of reaction for each of the four decision reactions are equal to their final concentrations.

A player can consider their range of expected pain (Δh_α) values given their pre-bias levels to determine how they will play. For example, Player A may want to minimize his own total pain (Δh_A), the difference between his and his opponent's pain (Δh_A-Δh_B), or the sum of his and his opponent's pain (Δh_A+Δh_B). As shown in Figure 7, given that Player B is selfish and playing with c_{0b1} = 0.5, Player A would minimize his or her own pain by showing a bias towards *tell* (i.e. c_{0a1} = 0), earning the lowest years of prison time. If A would rather minimize their combined pain, then A should show a bias towards *quiet* (i.e. c_{0a1} = 1.0). However, if A instead wishes to make the game most fair, by minimizing the difference between their pains, then A should play with a bias of c_{0a1} = 0.5. At this level of bias, both players receive the exact same pain. This analysis hints at an important moral question related to the dilemma between maximizing fairness and minimizing expected pain, as the overall welfare-maximizing outcome may not result in the most fair solution[19].

[19] Kaplow, L., Shavell, S. *Fairness Versus Welfare.* Harvard University Press. 2006.

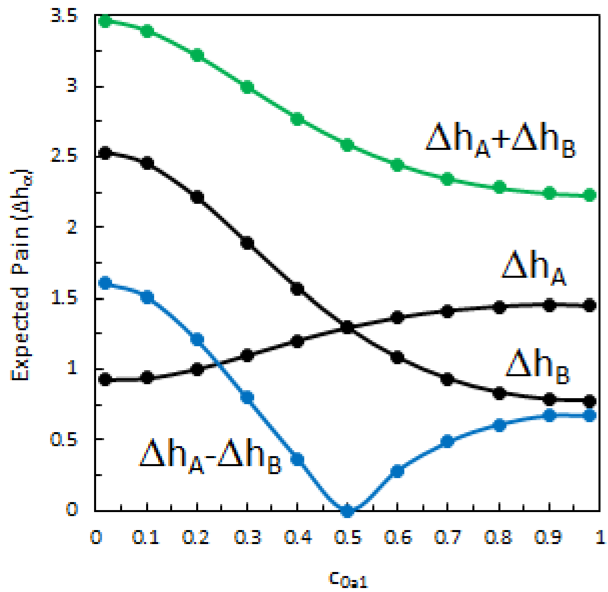

Figure 7. Expected Pain Values if Player B is Selfish and Unbiased
Expected Pains for Players A and B (Δh_A, Δh_B), sum of pains (Δh_A+Δh_B), and difference of pains (Δh_A-Δh_B). c_{0b1} is held constant at 0.5. For the difference of pains curve, there is a differentiable minimum at c0a1 = 0.50. Two unbiased players (c_{0a1} = c_{0b1} = 0.5) give the most equal outcome (minimum Δh_A-Δh_B), but a Player A biased towards *tell* yields the lowest total pain (minimum Δh_A+Δh_B).

However, as another example, if B is still unbiased but playing with an *overall* perspective, Player A would consider his strategy differently. As shown in Figure 8, if A wants a fair outcome, he can play with c_{0a1} = 0.8. Again, the two players receive the exact same pain here. If A wants to minimize his own pain, he can play with c_{0a1} = 0. Notice that player B receives a very high pain on this end of the graph - higher than he would have received if he played selfishly. This is the risk of playing overall: If Player A takes advantage of Player B’s strategy, Player B has a possibility of incurring a very high pain. And finally, if A wants to minimize the total pain of both players, he can play with c_{0a1} = 1. Notice that the combined pain here is less than that in Figure 8a. This is the benefit of playing overall: If Player B plays overall and Player A also attempts to minimize their combined total pain, both players do better than they would have playing selfishly.

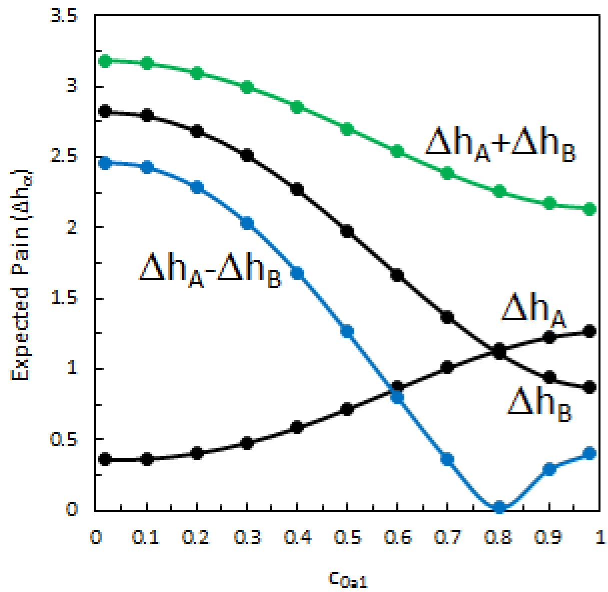

Figure 8. Expected Pain Values if Player B plays Overall and Unbiased
If both players adopt a strategy that focuses on maximizing the welfare of the group, they do better than playing selfishly.

As a final example, A can consider how he will play if he knows B is selfish but biased either towards *tell* (c_{0a1} = 0.1) or towards *quiet* (c_{0a1} = 0.9). Figure 9a details the results if Player B is biased towards *tell*. In this case, if A wants to ensure a fair outcome, he can - like Player B - play with a bias of c_{0a1} = 0.1 (also biased towards tell). Player A’s pain is minimized on this end of the graph, where c_{0a1} is close to 0. However, if A wants to minimize their combined pain, he does best playing with a bias of c_{0a1} = 1. Thus, when a player knows their opponent will pick *tell*, their best strategy for themselves is to pick *tell* as well. This is very similar to solving for the Nash equilibria in classical game theory: Classical players know their opponent will pick tell if they are “rational,” and thus they should pick tell themselves. Here, a player’s disposition towards tell is explained by their pre-bias, rather than rationality.

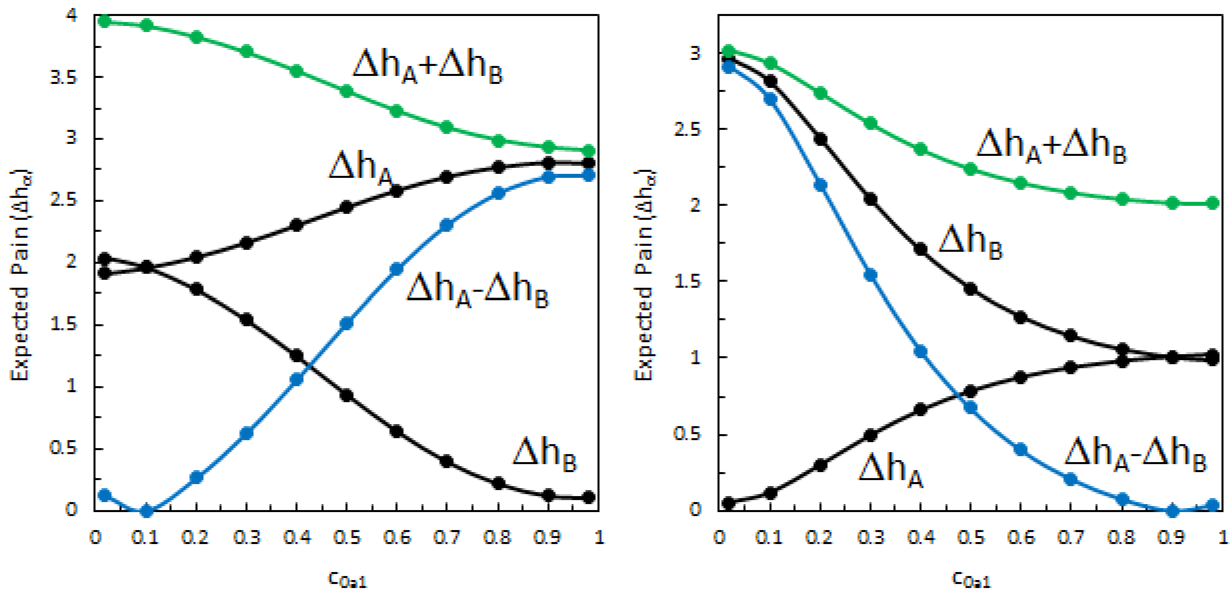

Figure 9. Expected Pain Values if Player B is Selfish and Biased.
Figure 9a (left) shows the outcomes for a player with bias of $c_{0a1} = 0.1$ (biased towards tell). Figure 9b (right) shows the outcomes for a player with bias of $c_{0a1} = 0.9$ (biased towards quiet). In both cases, Player A does best for himself by adopting his opponent's level of bias. In all four graphs, there is a differentiable minimum where $\Delta h_A - \Delta h_B = 0$.

Figure 9b details the results if Player B is biased towards *quiet*. In this case, if A wants to ensure a fair outcome, he can - like Player B - play with a bias of $c_{0a1} = 0.9$ (also biased towards quiet). If Player A wants to minimize his own pain, he should play with a bias of $c_{0a1} = 0$. The difference between the pains on this end of the graph is particularly large because Player B has a possibility of incurring a very high pain if player A takes advantage of them and picks *tell*. Like playing overall, playing with a high pre-bias towards *quiet* is a risk. However, if A wants to minimize their combined pain, he does best playing with a bias of $c_{0a1} = 1$. The lowest possible combined pain of Figures 7-9 occurs here, if Player A also plays with this bias towards *quiet*. This graph helps illustrate the concept of trust: Players likely play with a bias towards *quiet* because they trust that their opponent seeks to help them as well. If their opponent does help them, they get the best outcome possible, where their pain is minimized. And if their opponent does not, they learn through the experience to change their pre-bias and perspective to lower their total pain.

This exercise could be done for a number of scenarios, but these examples illustrate how players can maximize their own welfare, total welfare, and fairness, given the pre-bias and perspective of their partner. This approach is more complicated than finding best responses by inspection of a pain matrix. By considering their opponent's strategy and their goals for the outcome, players can determine how they wish to play.

Chapter 6

Conclusion

Earlier, this thesis listed four critical shortcomings of classical game theory, and showed in each section of Chapter 4 how CGT addresses them. To summarize:

1) The 100% problem. Classical game theory proposes that the {*tell, tell*} solution occurs 100% of the time, since players consider only their best response, and no information about the other player. However, this outcome almost never occurs experimentally. In CGT, there are never 100% solutions due to entropy, and the solution to games yield equilibrium mole fractions that represent how often each of the four decisions are expected to occur.

2) The Epsilon problem. If a PD game were played with pains that differed from each other by only a very small amount (ε=0.01), classical game theory predicts that players would still choose the {*tell, tell*} solution 100% of the time. However, for small differences, it was postulated that the solution would be more equally spread among the possible outcomes. This is the case for CGT solutions, as shown in Figure 3.

3) The Rationality problem. Classical game theory has not been able to explain experimental deviations from "rationality," those instances where players do not always act in way that maximizes their own utility. CGT readily allows for the incorporation of bias, trust, and perspective to account for these deviations. Furthermore, CGT acknowledges that deviations from rationality are not mistakes, but rather a result of the different personalities, information, and experiences that each player brings to the game.

4) The Decider problem. Chemical game theory allows readily for decider attributes through the D reactor. Figure 4 shows how the decider's perspective can change the equilibrium outcome of the game. For other common classical game theory models, such as Tragedy of the Commons, a decider could represent a type of enforcement mechanism. It is important to consider these outside agents and systems to determine how real games will be played.

CGT allows for analysis of the relative effects of the game's components - pain magnitudes, decider biases, player pre-biases, and player perspectives - on equilibrium outcomes. When pain magnitudes are moved closer together, players choose the four decisions with similar frequency, whereas in classical game theory, a 100% solution would still be attained. When all four pains are equal, the choice is totally entropic, and entropy aims to distribute the pains equally. CGT also incorporates the attributes of a decider, by allowing the district attorney to favor one decision over another. A decider that is significantly biased can have an important impact on the outcome, allowing any of the four decisions to dominate.

CGT also introduces pre-bias, which changes the initial concentrations of choice species a1, a2, b1, and b2. Pre-bias is one of the most impactful game attributes because, for example, when $c_{0a1} = c_{0b1} \approx 0$, it is not possible for D11 to dominate, no matter how favorable the choice is energetically. The idea of entropic choices is also important here, as the D22 decision will still never be a 100% solution, and D11 will still occur some small fraction of the time. And finally, CGT introduces perspective, which aims to account for how a player feels about their opponent's outcome by incorporating their opponent's $g_{\alpha\mathrm{ij}}$ value, either favorably or unfavorably.

Real players who know their opponent's strategy can decide how they wish to play the game, depending on whether they want to minimize total pain, minimize their own pain, or maximize fairness of the outcome. The role of trust is important here because a player incurs a high pain if their trust is taken advantage of, but two trusting players can achieve the lowest total pain outcome, by playing overall and with a bias towards *quiet*.

Future work in CGT can focus on the effects of temperature and pressure on the outcomes of decision reactions. This thesis assumed standard temperature and pressure, an assumption which is easy to change mathematically, but it is more difficult to define what these terms mean behaviorally. Another important area of future work is solving networks of chemical reactions kinetically, instead of as equilibrium reactions, as the dynamic effects (such as the time required to process each decision) may be important in understanding outcomes. Additionally, this thesis focused only on two-player games. However, it is not uncommon to have classical games with three or more players, each with three or more choices. It is important to repeat this analysis for larger sets of players and choices and compare the results to a wider variety of experimental data in order to test the validity of CGT results.

The approaches of CGT admit the possibility of using concepts from chemistry and chemical engineering to predict outcomes of decision-making in social systems. Classical game theory is normative and indicates what a rational player should do. But science does not tell us what *should* happen; rather, it tells us what *will* happen. Grounded in scientific principles, CGT seeks to be descriptive and predict how real players will behave. Understanding this behavior can allow us to engineer our environments, whether altering the energetics of certain choices, strengthening enforcement mechanisms, or biasing players towards particular decisions, to generate outcomes that offer greater benefits for all.

Appendix A

Thermodynamic Derivation

This derivation follows Denbigh[20], and begins with the thermodynamic equation:

$$dG = -SdT + VdP + \sum \mu_i dn_i$$

Where G is the Gibbs free energy, S is the entropy, T is the temperature, p is the pressure, V is the volume, μ_i is the chemical potential of species i, and n_i is the moles of species i. If the reaction occurs at constant T and p, so that dT = 0 and dp = 0, this simplifies to:

$$dG = \sum \mu_i dn_i$$

The reaction coefficients (ν_i) are set by the stoichiometry. The change in moles for each species can be expressed in terms of an extent of reaction (ε), as

$$dn_i = v_i d\varepsilon$$

Using a general expression for chemical potential, with units of J/mol: $\mu_i = \mu_i^0 + RTln a_i$, the Gibbs free energy can be expressed as:

$$dG = \sum (\mu_i^0 + RTln a_i)\, v_i d\varepsilon$$

The activity of a gas phase molecule is $a_i = y_i\, \phi_i\, (p/p^0)$, at a pressure p and standard pressure p^0, where y_i is the mole fraction of species i, including all inert species. If the pressure is not too high, the gas will be approximately ideal, so that the fugacity coefficients $\phi_i \approx 1$. The Gibbs free energy varies with the extent of reaction (ε), and to find the equilibrium extent, one can minimize the Gibbs free energy by setting the derivative with respect to ε equal to 0.

By definition the standard state Gibbs energy change of reaction is:

[20] Denbigh, Kenneth. *The Principles of Chemical Equilibrium*, 4th ed, Cambridge University Press (1981).

$$\Delta g^0 = \sum \mu_i^0 \, v_i$$

Which gives the expression shown in Equation 4:

$$\Delta g^0 = -RT \ln\left(\frac{p}{p^0}\right) \sum v_i - RT \sum v_i \ln y_i$$

Appendix B

Excel Solver Example

Player A (self)		guess		
eps1	0.06246	0.05666		
eps2	0.00117	0.00106		
eps3	0.13933	0.12338		
eps4	0.0026	0.00241		
species	initial	change	end	y mole frxn
a1	0.5	-0.0636	0.43637	0.2431792
a2	0.5	-0.1419	0.35808	0.1995463
b1	0.9	-0.2018	0.69821	0.3890957
b2	0.1	-0.0038	0.09624	0.0536298
A11	0	0.06246	0.06246	0.0348087
A12	0	0.00117	0.00117	0.0006493
A21	0	0.13933	0.13933	0.0776426
A22	0	0.0026	0.0026	0.0014483
inert	0	0	0	0
SUM	2	-0.2056	1.79445	1
eq	Dg0/RT	-SUM(nui ln yi)		dif^2
1	1	1		1.89E-17
2	3	3		3.546E-20
3	0	2.8E-09		7.847E-18
4	2	2		4.958E-18
				3.174E-17

Player B (estimate)		guess		
eps1	0.0662516	0.06294		
eps2	0.0174531	0.0163		
eps3	0.0104837	0.01001		
eps4	0.0027618	0.00266		
species	initial	change	end	y mole frxn
a1	0.5	-0.0837	0.4163	0.21875166
a2	0.5	-0.0132	0.48675	0.25577601
b1	0.9	-0.0767	0.82326	0.43260281
b2	0.1	-0.0202	0.07979	0.04192485
B11	0	0.06625	0.06625	0.03481338
B12	0	0.01745	0.01745	0.00917113
B21	0	0.01048	0.01048	0.00550891
B22	0	0.00276	0.00276	0.00145125
inert	0	0	0	0
SUM	2	-0.097	1.90305	1
eq	Dg0/RT	-SUM(nui ln yi)		dif^2
5	1	1		1.353E-17
6	0	1E-09		1.0047E-18
7	3	3		2.7444E-18
8	2	2		1.621E-21
				1.7281E-17

Player D (estimate)		guess		
eps1	0.0196235	0.01724		
eps2	0.0001691	0.00016		
eps3	0.005946	0.00559		
eps4	6.703E-05	6.2E-05		
species	**initial**	**change**	**end**	**y mole frxn**
A11	0.0624625	-0.0196	0.04284	0.1548228
A12	0.0011651	-0.0002	0.001	0.0035997
A21	0.1393256	-0.0059	0.13338	0.4820427
A22	0.0025989	-7E-05	0.00253	0.0091504
B11	0.0662516	-0.0196	0.04663	0.1685169
B12	0.0174531	-0.0002	0.01728	0.0624655
B21	0.0104837	-0.0059	0.00454	0.0163998
B22	0.0027618	-7E-05	0.00269	0.0097391
D11	0	0.01962	0.01962	0.0709207
D12	0	0.00017	0.00017	0.0006112
D21	0	0.00595	0.00595	0.0214891
D22	0	6.7E-05	6.7E-05	0.0002422
inert	0	0	0	0
SUM	0.3025024	-0.0258	0.2767	1
eq	**Dg0/RT**	**-SUM(nui ln yi)**		**dif^2**
9	-1	-1		8.958E-18
10	-1	-1		3.908E-18
11	-1	-1		6.352E-23
12	-1	-1		2.48E-19
			SUM	1.311E-17

	actual	**fraction**
a1	0.147332	0.487045
a2	0.15517	0.512955
b1	0.278523	0.920731
b2	0.023979	0.079269
D11	0.019624	0.760435
D12	0.000169	0.006554
D21	0.005946	0.230413
D22	6.7E-05	0.002597

Appendix C

Perspective Game Matrices

Player B is rivalrous:

	b1 = quiet	b2 = tell
a1 = quiet	***1***, 0	***3***, *-1.5*
a2 = tell	***0***, *1.5*	***2***, 0

Player B is altruistic:

	b1 = quiet	b2 = tell
a1 = quiet	***1***, 1	***3***, 3
a2 = tell	***0***, 0	***2***, 2

Player B is vengeful:

	b1 = quiet	b2 = tell
a1 = quiet	***1***, -1	***3***, -3
a2 = tell	***0***, 0	***2***, -2

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Academic Vita

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EDUCATION

The Pennsylvania State University, University Park, PA
Schreyer Honors College
Bachelor of Science in Chemical Engineering, Minor in Economics **–** *May 2018*

National University of Singapore, Singapore
University Scholars Program, Department of Chemical Engineering – *Jan - May 2017*

WORK EXPERIENCE

Velegol Lab, Department of Chemical Engineering, State College, PA – *Aug 2015* **-** *Present*
Undergraduate Research Assistant, Chemical Game Theory

- Analyze collective decision-making processes in social systems using chemical engineering principles, including thermodynamics and chemical equilibria
- Use Microsoft Excel and Mathematica to quantify strategies for human decision-making
- Wrote op-ed based on research that was published in the *Pittsburgh Post-Gazette*
- Served as a teaching assistant for a class of 90 students pertaining to research subjects
- Presented research at the 2016 AIChE National Convention and in chemical engineering classes

Shell, Puget Sound, WA – *May* **-** *Aug 2017*
Process Engineering Intern, Downstream Refining

- Created a process flow diagram and thermodynamic monitoring tool for a refinery steam system
- Worked with teams in operations and utilities to implement its use in daily monitoring processes
- Designed an Excel tool to compare computer projections for stream qualities with lab samples
- Consulted with crude schedulers and economists to use results to update software inputs and biases
- Presented to process engineering department and at a webinar for interns across the U.S.

Penn State Learning, State College, PA **–** *Aug 2015 – Dec 2016*
Guided Study Group Leader, Organic Chemistry

- Taught 3 hours at weekly sessions available to over 800 students enrolled in Organic Chemistry I
- Prepared PowerPoint presentations, practice problems, and learning strategies for students
- Recognized for having one of the highest attendance levels, with up to 320 students per session
- Consulted bi-weekly with course faculty and mentored new undergraduate teaching assistants
- Received the 2015 Outstanding Guided Study Group Leader Award

Dow Corning/Dow Performance Silicones, Midland, MI **–** *May* **-** *Aug 2016*
Science and Technology Intern, Engineered Materials

- Led project to qualify a new raw material source for two thermally conductive electronics products
- Manufactured pilot-scale batches and measured their rheological and thermal properties
- Managed scale-up to production equipment
- Recommended product formulation adjustments based on statistical analysis in Minitab
- Wrote technical report and presented project results to stakeholders

ACTIVITIES

American Institute of Chemical Engineers, Community Service Chair – *Sept 2014* **-** *Present*
Plan and assist with recruitment, mentoring, and outreach events for Penn State chemical engineers
Perform science workshops and demonstrations at local grade school and community events

Schreyer Honors College Orientation, Mentor – *Aug 2015, Aug 2016*
Led groups of 10-12 incoming honors engineering students through a 3-day orientation program

GLOBE Special Living Residence Hall, Member – *Aug 2014* **-** *Dec 2016*
Selected through an application process to live in a residence hall focusing on global issues
Hosted discussions and attended lectures and documentaries about international events

Penn State Campus Orchestra and Flute Choir, Flutist – *Sept 2014 – Dec 2016*

AWARDS

- NASA Pennsylvania Space Grant Consortium Undergraduate Scholarship
- Schreyer Honors College Academic Excellence Scholarship
- Penn State Engineering Scholarship and Provost Award