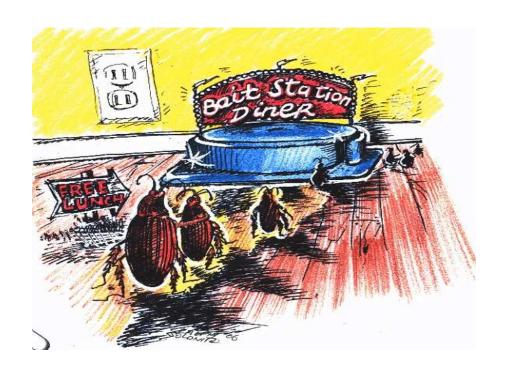
# Scent of a Woman: Application of Cockroach Pheromone as Bait



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#### **ABSTRACT**

The enclosed report addresses the possibility of integrating a synthetic roach sex pheromone into an existing trapping mechanism to produce a superior roach control product. This new product would be an off the shelf brand designed for private homeowners, and should be competitive with the current market leader, Maxforce.

It was decided to market this product in a gel form that combines the pheromone blattellaquinone and maltose as the attractants, fipronil as the active insecticide, and carrageenan as the gel matrix. The southwestern United States (TX, OK, KS, NV, AZ, NM, CA, UT, CO) is the target distribution area.

Utility functions were created to assess the necessary characteristics of the new product from a consumer standpoint. Four characteristics of the new product were rated by ten consumers through the distribution of surveys. The four characteristics were: durability, speed, odor, and toxicity. Each of these characteristics were then linked to an adjustable component of the new product such that shifting the composition of the product altered consumer satisfaction ratings accordingly.

The resulting utility functions were then used in combination with an economics based pricing model correlation to analyze how product composition affects supply and demand.

Maximizing the utility functions under reasonable constraints led to a product composition of 10mg/tube of fipronil, 0.02mg/tube of blattellaquinone, and 15000mg/tube maltose. These compositions correspond to a selling price for the new product of \$6/unit along with an expected demand of 2,500,000 units. At this selling price and demand the estimated NPV after 10 years was calculated to be \$90,000,000. The FCI and TCI are \$1,800,000 and \$2,200,000 respectively.

A more optimal solution was pursued with the utilization of risk and uncertainty, but this attempt proved unsuccessful. In the future, this avenue will be pursued thoroughly in an attempt to more confidently select a product composition. The unsuccessful attempts at incorporating risk are included in the report appendices.

Future work centers heavily on pursuing a more optimal solution using risk and uncertainty. In addition, the results of the utility functions depend heavily on the population model. To this end it would be advisable to make the model as accurate as possible for future calculations. Also, more accurate estimates are needed for the total revenue available in this narrow market because the estimated profit per year for this new product seems uncharacteristically large.

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#### **INTRODUCTION**

Cockroaches are one of the major sources of insect infestations in homes and businesses. Of the approximately 4000 known species of cockroaches, the most common is *Blattella germanica*, or the German cockroach<sup>13</sup>. Approximately 1.9cm long, the small size of the German cockroach allows it to easily hide in crevices and walls, making detection and extermination difficult. Infestations can escalate into serious problems quickly; a single German cockroach can produce up to 300,000 roaches in one year<sup>13</sup>.

Eliminating roaches is very important, as they pose a major health risk. Roaches travel about and eat any waste, including human and animal feces. This means they can easily transmit disease with viruses and bacteria. In fact, at least 100 species of bacteria have been isolated from cockroaches, such as *Salmonella*, *E. coli*, and *Shigella*<sup>10</sup>. Furthermore, roaches can carry house dust mites, powerful aggravators of asthma<sup>10</sup>.

Because of this dangerous health hazard, it is imperative to develop new techniques to challenge the roach problem. In February of 2005, Dr. Wendell L. Roelofs and his team published groundbreaking research. Using advanced and modified chromatographic techniques, the volatile sex pheromone of German cockroaches was isolated and successfully synthesized<sup>11</sup>. Termed "blattellaquinone", this discovery proves to be a powerful attractant for male German roaches<sup>11</sup>.

#### **OBJECTIVE**

It is proposed that by incorporating blattellaquinone into a roach trap, an effective method for quelling roach infestations is possible. This project seeks to develop such a device. The scope of this research will encompass the composition of the new product, the design of the process plant needed for efficient production, and the economics to make such a product profitable as well as competitive in the roach bait market.

#### PHEROMONE SYNTHESIS

The female sex pheromone for *Blatella Germanica* was isolated by a group of researchers at Cornell University. This pheromone was a challenge for researchers to isolate because of the small amounts actually secreted by the female, and the substantial thermal instability of the pheromone itself. It was so difficult that many experts doubted its existence.

The final successful isolation procedure utilized several different chromatographic and separation techniques. Gas-chromatographic electroantennogram detection (GC-EAD), Silica Gel Separation, Nuclear Magnetic Resonance Characterization, High Performance Liquid Chromatography, and Gas-chromatograph Mass Spectrometry were a few of the techniques employed.

The artificially synthesized pheromone is very promising as an attractant. In field tests at a roach infested pig farm  $10\text{-}100\mu g$  of pheromone trapped 10-30 cockroaches per night. In lab tests 10-100ng attracted 60% of the males.

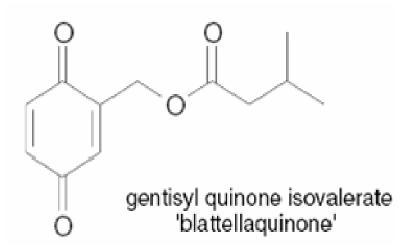


Figure 1: Blattellaquinone<sup>11</sup>

#### **PRODUCT DESIGN**

There were several possible choices on how to capitalize on the synthesis of blattellaquinone. Products that claim to eliminate roach infestations come in aerosol, granular, bait station, bait gel, and homemade hybrid apparatus forms. Obviously, each supplier claims that his/her method for trapping roaches is superior to all the others. From the research the research conducted it was decided that a roach bait gel was the optimal delivery vector for the poison and pheromone. A roach bait gel would maximize effectiveness without having the downsides of the other types of bait.

Aerosol insecticides are great for making people feel better but are not that effective against roach infestations. This is because aerosols can only kill the roaches that are not hidden very well, so that all the roaches inside the walls get away. Thus, the infestation is back in full force fairly quickly. Granular roach baits would be a good choice, but they can not be eaten by the roach nymphs. And since roaches reproduce like crazy, for large infestations a substantial portion of the roach population can not take the bait, creating an incomplete extermination. Bait stations are operationally the best but they have drawbacks in that they are hazards to children and pets. Thus, bait stations have to be placed very carefully creating hassle for consumers.

This leaves only the bait gels. Bait gels can be applied to cracks and crevices, nymphs can eat them, and they can be placed anywhere at the consumer's discretion. Combining an insecticide with the bait gels makes them as efficient at removing infestations as any other method.

The active insecticide chosen for application in the roach bait gel is fipronil. Fipronil is part of a newer class of poisons that tends to kill more slowly than typical insecticides. This is a desirable quality in an insecticide targeted towards roaches because many other roach poisons tend to kill too quickly. This does not give the poison a chance to thoroughly spread through the population. Fipronil has a delayed effect, allowing roaches who are infected to pass it on to other roaches in the colony.

Blattellaquinone is the prototype aspect of the new product that will hopefully increase its effectiveness. Being a sex pheromone, the addition of blattellaquinone to a roach bait gel should theoretically increase the amount of males attracted to the bait. For this reason the pheromone can not be the only attractant used, or the females and nymphs will never approach it. In addition to the sex pheromone a traditional sugar based bait attractant is used. Maltose is used so that the new product maintains the standard attractive power across the range of cockroach types.

Carrageenan gel is the last main component of the product. This gel is the matrix which holds all the other components. This gellant is a seaweed extract that is cheap and easy to acquire.

#### **MARKET SELECTION**

The target area for the new product will be the southwestern United States. These are the states of: Californian, Nevada, Utah, Arizona, Colorado, New Mexico, Kansas, Oklahoma, and Texas.



Figure 2: Target Area<sup>20</sup>

In addition to this, the new product will be an off the shelf roach bait gel for use in home infestations. Theoretically, it should also work for massive infestations of businesses, but this option has not been thoroughly explored.

#### **UTILITY FUNCTIONS**

Adequate design and pricing of a potential product must take into account the consumers' desires. To model consumer concerns and expectations utility functions are created. The purpose of a utility function is to link important product attributes to quantitative physical properties. To construct the necessary utility functions consumer surveys were distributed. These surveys were carefully crafted such that they yielded information necessary for the construction of the " $\beta$ " function (beta function). The  $\beta$  function represents consumer preference and its importance in the overall pricing model will be explained in more depth later.  $\beta$  is represented as a ratio of preferences in which  $S_1$  is the consumer satisfaction for the new product and  $S_2$  is the consumer satisfaction for the competitor's product. The goal is to minimize the beta function by maximizing the satisfaction for our product relative to that of our main competitor (Maxforce).

$$\beta = \frac{S_2}{S_1}$$

The satisfaction function "S" is given by the following formula:

$$(2) S_i = \sum_i w_i y_i$$

 $w_i$  represents the weighting factor for an attribute, and  $y_i$  represents the normalized score of a given consumer attribute. For the consumer model four attributes that affect the product quality were chosen:

- 1) Durability- How long is it before the roach problem returns?
- 2) Speed- How long does it take to reduce or eliminate the infestation?
- 3) Odor- How badly does it smell?

#### 4) Toxicity- How safe is it for people and pets?

This means that for any given product composition formula (2) has to be calculated 4 times, once for each attribute. The 4 results are then summed to yield the " $S_2$ " value in formula (1).

The first question on the survey prompted consumers to rank these 4 attributes from most important to least important in a roach killer product. This information was used to account for the fact that some attributes are more important than others.

- 1) Rank the following categories from most important "1" to least important "4" in a roach removal product:
  - a. Durability (How long is it before the roach problem returns?)-2
  - b. Speed (How long does it take to reduce or eliminate the infestation?)-3
  - c. Odor (How badly does it smell?)-4
  - d. Toxicity (Is it safe for pets and people?)-1

Some additional steps had to be taken in order to convert these consumer rankings into a useable format. The problem is that in order to use this information to find the "w" values in the preference function (formula 2), these numbers have to be converted into weight fractions. The following equation is used to accomplish this.

(3) 
$$w = \frac{n}{1+2+3+4}$$

"n" can equal 1, 2, 3, or 4 which correspond to possible weight fractions of 0.1, 0.2, 0.3, or 0.4 respectively (1/10, 2/10, 3/10, 4/10). Given these 4 choices of weight fractions it is clear that 0.4 is the heaviest weight and 0.1 is the lightest. What is not clear is that these weight fractions have an inverse correspondence to the consumer rankings. This means that if a consumer ranks toxicity as #1 (the most important), this is not a weight fraction of 0.1 like equation (3) would imply, but rather a weight fraction of 0.4. This can be understood by examining the data conceptually. The most important attribute should have the most impact on the preference function. In order to have the most impact an

attribute has to be weighted the heaviest out of the 4 weights available (0.4). With this logic, consumer rankings of 2, 3, and 4, correspond to weight fractions of 0.3, 0.2, and 0.1. The last step of this process is to realize that there were 10 consumer surveys; not just one. This means that in order to find final weight fractions for each attribute's importance an average had to be taken across all 10 surveys. Table 1 shows the final weight distributions for each attribute.

	1	2	3	4	5	6	7	8	9	10	Average weight
Durability	40%	10%	40%	20%	20%	10%	10%	10%	20%	10%	19%
Speed	20%	30%	30%	30%	30%	40%	40%	40%	30%	40%	33%
Odor	10%	20%	10%	10%	10%	30%	30%	20%	10%	20%	17%
Toxicity	30%	40%	20%	40%	40%	20%	20%	30%	40%	30%	31%

**Table 1: Weight Percents** 

From the table it can be seen that the consumers polled felt that speed was the most important aspect of a roach control product. Speed is closely followed by toxicity. Thus, when components are varied in the product the components that affect speed and toxicity will have the biggest impact on the  $\beta$  function.

Once the weight of each attribute ("w" value) is found from the surveys it does not change. The same can not be said for the "y" values because they will vary with product composition. The "y" in formula (2) is actually a normalized representation of consumer happiness. As the product composition changes so will the expected consumer happiness. "Y" values are not fully described here but are more thoroughly addressed in the following subsections. The goal is to, based on the data from the consumer surveys, construct a relationship between quantitative amounts of a given component, and the resulting normalized "y" value. In this way, changing the composition of the product will affect the beta function.

#### **DURABILITY**

As stated above, durability is a measure of the length of time it takes for your roach problem to return. Below are examples of the type of questions that were asked on the survey to begin modeling the durability utility function.

2) How satisfied would you be if the product permanently killed all the roaches the first time you used it?

3) How satisfied would you be if the product killed enough roaches so that you didn't see them anymore, but you had to repeat the process every 3-6 months?

The results from a total of 10 surveys were tabulated and compiled to create the following table:

DURABILITY		Satisfaction Ratings per survey #									
	1	1 2 3 4 5 6 7 8 9 10							Average		
Permanent roach death	100%	100%	100%	100%	100%	100%	100%	100%	100%	100%	100%
3-6 month roach lull	60%	80%	60%	20%	60%	100%	60%	60%	100%	40%	64%
1 month roach											
reprieve	0%	0%	0%	0%	0%	80%	40%	40%	40%	20%	22%

**Table 2: Durability Information** 

It can be seen from the survey that mathematically speaking a rating of "1" should correspond to a 20% consumer satisfaction rating, but it was decided that a rating of "1" should be normalized to 0% satisfaction while leaving a rating of "5" at 100%. Table 1 illustrates the results of the raw data collected but does not illustrate the data actually used to construct the utility function. A few modifications had to be made to the data for the purposes of implementation. The durability function actually depends on 3 different

parameters; the amounts of blattellaquinone, fipronil, and maltose. To account for this multi-parameter dependence a complex population model had to be created. The creation and explanation of this population model is contained later in the report; after which the durability utility can be more fully explained. The following table graphically shows the relationship between a given result and consumer happiness with that result.

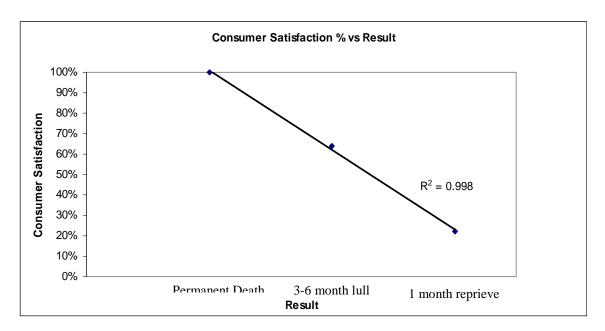


Figure 3: Consumer Satisfaction versus Result

#### **SPEED**

Speed is the category that addresses how long it takes for the consumer to see results. This is very important because many people have thresholds for how long they are willing to wait for a result. The following is an example of question asked on the survey in the speed category.

# 5) How satisfied would you be if the product eliminated your infestation in 24-48 hours? 1 2 3 4 5 (not satisfied) (very satisfied)

The survey tested people's preferences in the time periods of 1-2 days, 3-4 days, 5-7 days, and 1-2 weeks. This delineation makes the assumption that almost no one will be happy if eliminating a roach problem takes more than 2 weeks, and the data collected confirms this.

The construction of this utility function is almost identical to the procedure used to construct the durability function. Speed also depends on maltose, fipronil, and blattellaquinone. How speed contributes to the  $\beta$  function will also be left until after the population model has been explained. The following tables show the initial data collected in the speed category.

SPEED		Satisfaction Ratings per survey #									
	1	2	3	4	5	6	7	8	9	10	Average
24-48hr elimination	100%	100%	80%	80%	100%	100%	100%	100%	100%	80%	94%
3-4 day elimination	100%	40%	60%	60%	80%	80%	80%	80%	60%	60%	70%
5-7 day elimination	80%	0%	40%	40%	60%	40%	40%	60%	40%	40%	44%
1-2 week elimination	60%	0%	0%	0%	0%	0%	0%	0%	0%	0%	6%

**Table 3: Speed Survey Data** 

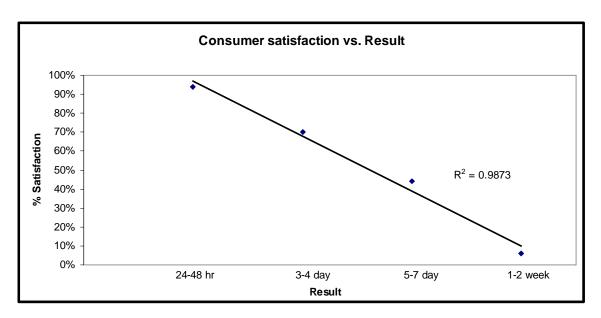


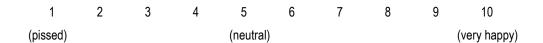
Figure 4: Satisfaction versus Result

#### **ODOR**

Beyond sifting through the components of the new product to determine which components had a smell, constructing the odor utility function was straightforward. There was no need to use the population model that needed to be constructed for the durability and speed utilities. The roach bait gel can be simplified to 4 main components which could contribute to the smell of the final product: the carrageenan gel matrix, maltose, fipronil, and blattellaquinone. From material safety data sheets (MSDS's) it was determined that carrageenan and maltose have no discernable smell, while fipronil has a slight sweet odor. As far as can be determined blattellaquinone does not have a smell, but this is not a certainty given its new-found status as a mass market product. No smell was reported during pilot scale tests, but a roach bait gel will be utilizing substantially larger amounts. For calculation purposes the pheromone was assumed to have no discernible smell. This means that the only component that affects the smell is the fipronil.

The odor section of the survey changed the form of the questions slightly. The difference is that these questions were rated on a scale from 1 to 10 instead of from 1 to 5. There was no strategic reason for this change, other than to experiment with possible increased accuracy in the surveys.

#### 9) How happy would you be if the product had a very slight, unpleasant or odd, odor?



Once again the data from 10 surveys were compiled and averaged.

ODOR		Satisfaction Ratings per survey #									
	1	2	3	4	5	6	7	8	9	10	Average
slight odor	40%	50%	80%	50%	50%	40%	50%	80%	50%	50%	54%
odorless	100%	100%	100%	100%	100%	80%	100%	100%	100%	90%	97%
moderate odor	20%	0%	30%	50%	30%	30%	30%	40%	30%	40%	30%
overpowering stench	0%	0%	0%	40%	0%	20%	0%	20%	0%	20%	10%
pleasant fragrance	40%	40%	90%	100%	60%	100%	90%	60%	70%	50%	70%

Table 4: Odor Data

From the fipronil MSDS the following information was gathered in regards to the amounts of fipronil that produce a given reaction in the general population.

<u>POISON</u>	Fipronil (mg/tube)	Avg. Satisfaction
slight odor	200	54%
odorless	0	97%
moderate odor	400	30%
overpowering stench	1000	10%

Table 5: Amount of Poison for a given Result

Graphing the results depicted in the two previous tables gives:

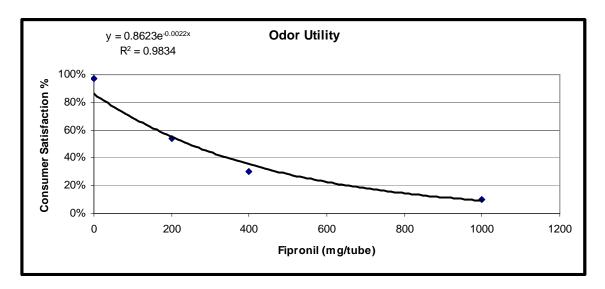


Figure 5: Odor Utility

The exponential equation fit to the data points makes it possible to find a consumer satisfaction percentage for any given input value of fipronil.

#### **TOXICITY**

Toxicity is the most important aspect of the potential new product and depends only on fipronil. Even though speed had a slightly higher average weight, consumers still rated this attribute a very close second. This is the category where the absolute maximum allowable amounts of fipronil are set. A startup company with any reasonable hopes of succeeding can not afford killing people or pets, even if the product kills all the roaches too. So, to stay on the safe side at least an order of magnitude less than anything approaching a lethal dosage was used.

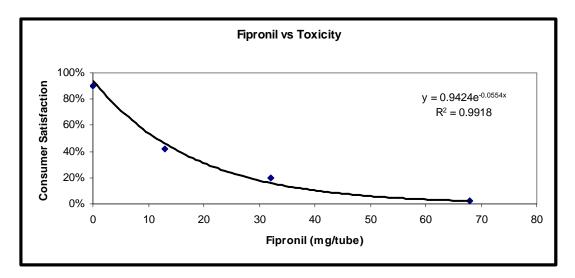
TOXICITY		Satisfaction Ratings per survey #									
_	1	2	3	4	5	6	7	8	9	10	Average
slightly toxic	60%	0%	60%	0%	20%	100%	40%	40%	80%	20%	42%
moderately toxic	40%	0%	40%	0%	0%	40%	20%	20%	40%	0%	20%
extremely toxic	20%	0%	0%	0%	0%	0%	0%	0%	0%	0%	2%
non-toxic	80%	80%	80%	80%	80%	100%	100%	100%	100%	100%	90%

Table 6: Toxicity data

To determine what amounts of fipronil correspond to the nebulous designations of "slightly toxic", "moderately toxic", etc... extensive LD50 information was analyzed. An LD50 number is the lethal dosage to kill 50% of a test population measured in units of (mass of poison administered)/(unit mass of test subjects). In all relevant LD50 articles regarding the toxicity of fipronil rats were used as the test subjects. The assumption was made that these numbers are accurate representations of human responses as well. For a "slightly toxic designation" a unit mass of 5 pounds was used. In other words, the amount of fipronil necessary to have a 50/50 chance of killing a creature 5 pounds in weight was used. 15 pounds was used for "moderately toxic" and 30 pounds was used for "extremely toxic".

POISON	Fipronil (mg/tube)	Avg. Satisfaction
slightly toxic	13	42%
moderately toxic	32	20%
extremely toxic	68	2%
non-toxic	0	90%

Table 7: Fipronil Amt. for a Given Result



**Figure 6: Toxicity Utility** 

The toxicity function was fit to an exponential equation. It should be noted that table 7 is in terms of mg/tube. This means that to even have a chance of being fatal, something close to 5 pounds would have to consume an entire tube of the roach bait gel.

Before the 4 utility functions can be combined to find an optimum  $\beta$  function the population model must be explained.

#### **POPULATION MODEL**

In order to efficiently design a roach bait product, the population dynamics of a roach infestation must be known. Thus, a mathematical model must be derived as to predict roach population behavior. With the model in place, various amounts of blattellaquinone,

maltose, and fipronil can be adjusted, revealing the effects that each has on the roach colony.

To begin the model, the basic equation for population change 18 is applied.

$$\frac{dTotal\ Population}{dt} = \left\{ Birth\ Rate \right\} - \left\{ Death\ Rate \right\}$$

**Equation 4: Change in Total Population** 

Simply stated, the change in a population is equal to the birth rate minus the death rate. If the death rate is higher than the birth rate, the population change is negative, and that population will become extinct.

In any roach colony, the population consists of three classes: adult males, adult females, and babies (nymphs). Therefore, the total population change consists of three differential equations.

$$\frac{dBabies}{dt} = (\#Females) \left( \frac{\#EggsLaid}{Female \cdot Time} \right) (SexRatio) - k_m (Babies)$$

**Equation 5: Change in Nymphs (Babies)** 

The change in the amounts of babies in a colony is related to the amount of births per time and the maturation rate. The birth rate is the number of eggs laid per female per unit time. This is multiplied by the number of females to give the total eggs laid per population. The sex ratio is the proportion of the number of males to females. In the event that the adult male population drops very low, the number of births will decrease.

It is also assumed here that the moment an egg is laid, it is considered part of the baby population. The time it takes to hatch and mature is included in the maturation factor, or

 $k_{\rm m}$ . The maturation factor is the rate at which a baby matures into an adult. Thus, as soon as the baby matures into an adult, it is no longer classified as a baby. One last assumption for this equation is that all babies reach maturity.

Next, the change in the adult population is considered.

$$\frac{dAdultMales}{dt} = \frac{k_m(Babies)}{2} - (NaturalDeathRate)(Males)$$

**Equation 6: Change in Adult Males** 

$$\frac{dAdultFemales}{dt} = \frac{k_m(Babies)}{2} - (NaturalDeathRate)(Females)$$

**Equation 7: Change in Adult Females** 

The change in both adult populations is equal to the maturation rate of the babies, minus the natural death rate. It is assumed that for a given set of eggs, half will be male, and half will be female<sup>19</sup>. The natural death rate is the rate at which the adults die as a result of old age, which is typically around 100 days for a German cockroach<sup>13</sup>.

Applying these equations to Microsoft Excel and starting with one adult male and one adult female, the following graph is generated.

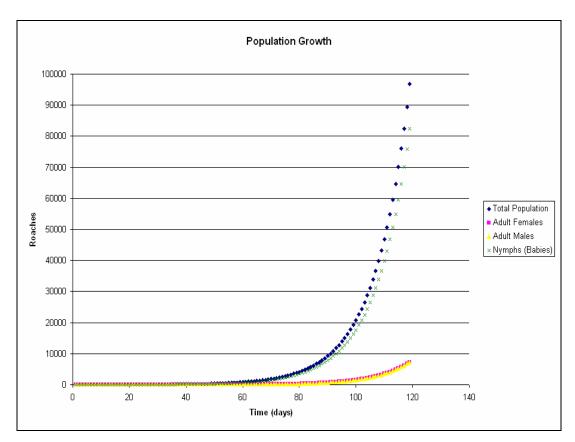


Figure 7: Change in Roach Population with Time

While roach populations do grow exponentially, it is not likely that it will grow to infinity. As with all populations, the roach colony will encounter limits, such as low food supply and limited space. In order to have an effective model, these factors must be incorporated.

The following are modifications to the growth equations:

$$\frac{d(AdultMales)}{dt} = \frac{km(Babies)}{2} - k_{natural death}(AdultMales) - k_{lack\ of\ food}AdultMales - k_{crowding\ effects}AdultMales$$

**Equation 8: Change in Adult Male Population** 

$$\frac{d(AdultFemales)}{dt} = \frac{km(Babies)}{2} - k_{natural death}(AdultFemales) - k_{lack\ of\ food} \\ AdultFemales - k_{crowding\ effects} \\ AdultFemales$$

**Equation 9: Change in Adult Female Population** 

$$\frac{dBabies}{dt} = (\# Females) \left( \frac{\# EggsLaid}{Female \cdot Time} \right) (SexRatio) - k_m (Babies) - k_{lack \ of \ food} Babies - k_{crowding \ effects} Babies$$

**Equation 10: Change in Nymph Population** 

The first new term,  $k_{lack \text{ of food}}$ , is the rate at which roaches die as a result of starvation. Because starving roaches die after about 30 days<sup>13</sup>, the value of this constant is varied until the roach population dies around 30 days. This occurs once the food supply is depleted. Thus, the model must also incorporate a food supply that diminishes as the roach population increases. The following is an equation that describes the change in food:

$$\frac{d(Food)}{dt} = -k_{consumption rate} * (Total Roaches)$$

**Equation 11: Change in Food** 

The constant  $k_{consumption\ rate}$  describes how much food one roach will eat in day. As the total amount of roaches in a colony increases, the food will decrease much faster. Because roaches do not consume much, it is assumed that one roach can eat approximately 0.8mg per day.

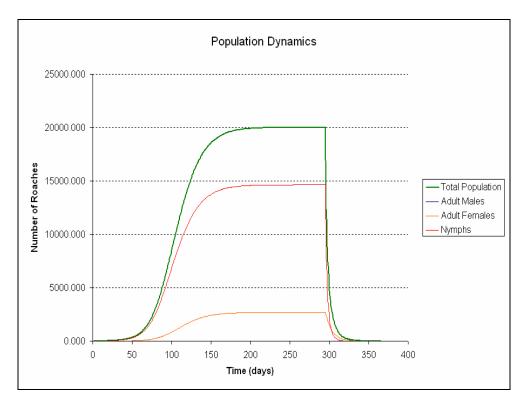
The next constant,  $k_{crowding\ effects}$ , describes how each population will change due to lack of space. This is proportional to the carrying capacity of the environment. Therefore, this constant is explained in the following:

$$k_{crowding\ effects} = k \frac{Total\ Roaches}{Carrying\ Capacity}$$

**Equation 12: Crowding Effects** 

As the population approaches the carrying capacity, this term becomes more significant. The constant 'k' in the equation describes how a roach will leave/die as a result of the lack of space. This equation is similar to the logistic equation for population growth<sup>18</sup>. This takes into account density effects, or the effect on population due to environmental limits.

The modified equations are applied to Excel, resulting in the following graph:



**Figure 8: Total Population Dynamics** 

This graph is much more reasonable. For the first 50 days, the roaches are becoming accustomed to the environment, but not growing to their full potential. During the next 100 days, the roaches are fully utilizing the environment and breeding at their maximum rate. By day 150, the population begins to reach the maximum capacity. This value is approximately 20,000 roaches in this case, a reasonable number for a typical cockroach infestation<sup>19</sup>. At the same time, roaches are continuing to feed. The change in food supply is shown in the following graph:

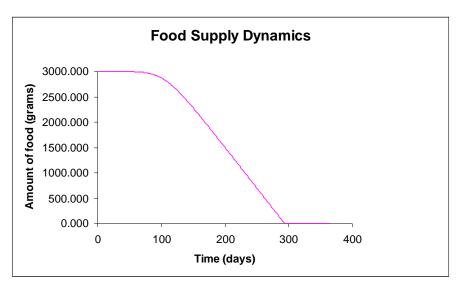


Figure 9: Change in Food Supply

Around day 300, the food supply is completely gone. Therefore, the roach population begins to starve and dies off around 30 days.

#### Adding Food

There is always the possibility that roaches will find additional sources of food.

Therefore, the population model is designed such that more food can be added for every specified number of days. The following illustrates how the user can adjust these parameters:

Population Model				
Constants				
Maturation rate	0.016666667			
Natural death rate	0.01			
Birth rate	1.142857143			
Roaches eat 'x' grams/day of Food	0.0008			
Roaches contact 'y' grams/day of Bait	0.008			
User Inputs				
Add poison on Day	1000			
Initial Food Supply (grams)	2000			
Add more food every 'x' days	30			
How many grams of food to add?	30			
Maximum Population	20000			

**Figure 10: Example of User Inputs** 

By adjusting the amount of food added, the effects on the roach population can be observed. The following chart depicts the effect of adding various amounts of food every 30 days:

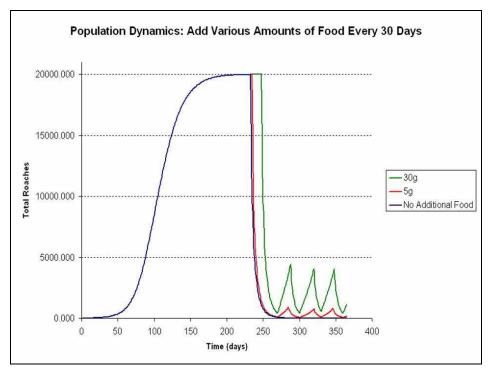


Figure 11: Adding Food Every 30 Days

It is clear that by adding more food, the population can be sustained for a greater amount of time. However, not adding enough food will still kill off a good portion of the colony. The spikes in the graph indicate that adding small increments of food will allow the roach population to grow slightly, but not enough to cause a major infestation.

#### Adding Poison to Model

With the core of the population model in place, the effects of the gel bait can now be included. The population is divided into three classes: noninfected, infected, and secondary infected. The noninfected roaches are the roaches having no contact with the poison. They grow and die at their natural rate until they are attracted to the gel. Once the roaches contact the bait, they are classified as infected roaches, dying at a rate proportional to the amount of poison. The final class deals with secondary infection. A noninfected roach can come into contact with an infected roach, whether it occurs through social interactions or cannibalism<sup>4,6</sup>. The poison transferred is still lethal, but the dosage will kill at a lower rate.

For simplicity, the nomenclature of each roach class is changed, as represented by the following table:

NonInfected	Infected	<b>Secondary Infected</b>
Adult Males	Adult Males	Adult Males
(NIM)	(IM)	(SIM)
Adult Females	Adult Females	Adult Females
(NIF)	(IF)	(SIF)
Babies	Babies	Babies
(NIB)	(IB)	(SIB)

**Table 8: Change in Nomenclature** 

The population change must now be described with nine different equations.

#### NonInfected Roaches

The first set of equations describes the change in the noninfected roaches. Using the same equation as described earlier with the modified nomenclature, three more terms are added.

$$\frac{d(NIM)}{dt} = \frac{km(NIB)}{2} - k_{natural death}(NIM) - k_{lack \ of \ food}NIM - k_{crowding \ effects}NIM$$

$$-k_{pheromone}NIM - k_{maltose}NIM - k_{sec}NIM \left(\frac{Infected_{Total}}{Total Roaches}\right)$$

**Equation 13: Change in Noninfected Adult Males** 

The variable,  $k_{pheromone}$ , is the infection rate at which the male roaches are attracted to the pheromone. This value is proportional to the concentration of the blattellaquinone used in the bait. The next term,  $k_{maltose}$ , is the rate at which the males are attracted to the maltose. This value is proportional to the concentration of maltose. The final term,  $k_{sec}$ , is the rate at which male roaches are contaminated by means of secondary infection. This term depends on the ratio of total infected roaches to all the roaches in the colony. In other words, if there are a greater number of infected roaches, the chance of secondary infection increases.

These new terms are applied to the adult female and baby populations as well. The only difference is that neither population is attracted to the pheromone.

$$\frac{d(NIF)}{dt} = \frac{km(NIB)}{2} - k_{natural death}(NIF) - k_{lack \ of \ food} NIF - k_{crowding \ effects} NIF$$

$$-k_{maltose}NIF - k_{sec}NIF \left(\frac{Infected_{Total}}{TotalRoaches}\right)$$

**Equation 14: Change in Noninfected Adult Females** 

$$\frac{d(NIB)}{dt} = k_{Birth Rate}(NIF)(SexRatio) - km(NIB) - k_{lack of food}NIB - k_{crowding effects}NIB$$

$$-k_{maltose}NIB - k_{sec}NIB \left( \frac{Infected_{Total}}{TotalRoaches} \right)$$

**Equation 15: Change in Noninfected Adult Nymphs** 

To determine how many roaches are attracted to the gel, approximations are made from research articles.

The attractive power of blattellaquinone is described in the following figures:

Attraction to Blattellaquinone							
Lab Amount							
(µg)	%Males	Scaled Up Amount (µg)					
1.00E-05	20	0.0125					
1.00E-04	22	0.125					
1.00E-03	41	1.25					
1.00E-02	62	12.5					

**Table 9: Blattellaquinone Attraction** 

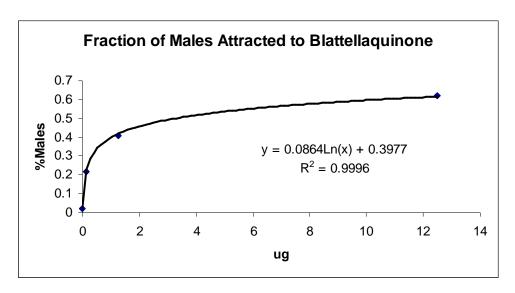


Figure 12: Percent Males Attracted to Various Concentrations of Pheromone

This trend was used to approximate the attractive power of blattellaquinone based on concentration. From table 9, increasing the concentration of blattellaquinone attracted more male roaches. Because this was in a lab setting with about 16 male roaches, such small amounts of pheromone may not have the same effect in a real infestation. Therefore, a simple proportion was set up, providing an estimate of the amount of pheromone to attract a colony of about 20,000 roaches. Furthermore, according to the Cornell University research, the percent of males attracted to the pheromone never exceeded 60%. Thus, the trend is set up to never attract more than 60% males.

The attractive power of maltose is presented in the following figures:

Maltose						
Grams	%Attr					
7	15					
20	32					
50	45					

**Table 10: Attraction to Maltose** 

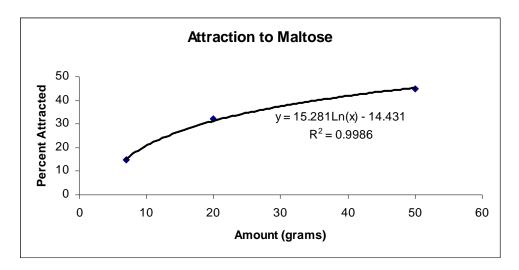


Figure 13: Attractive Power of Maltose

Research is slightly unclear as to the attractive power of maltose. While the roaches are attracted to this simple sugar<sup>1</sup>, the effect of concentrations is slightly unclear. Therefore, by including more sugar in the bait and assuming the bait will easily accessible to the roaches, it is assumed that more foraging roaches will be attracted.

#### Infected Roaches

As soon as the roaches come into contact with the bait, they are classified as infected. The following equations describe the change in infected roaches per time:

$$\frac{dIM}{dt} = \left(k_{pher}NIM\right) + \left(k_{maltose}NIM\right) - \left(k_{fipronil}IM\right)$$

**Equation 16: Change in Infected Males** 

$$\frac{dIF}{dt} = \left(k_{maltose} NIF\right) - \left(k_{fipronil} IF\right)$$

**Equation 17: Change in Infected Females** 

$$\frac{dIB}{dt} = \left(k_{maltose} NIB\right) - \left(k_{fipronil} IB\right)$$

**Equation 18: Change in Infected Babies** 

As stated earlier,  $k_{pheromone}$  and  $k_{maltose}$  describe the attractive power of the pheromone and maltose, respectively. The new term,  $k_{fipronil}$ , is the death rate of the roaches proportional to the concentration of fipronil in the bait. The death rates based on concentration are related in the following figures:

Fipronil		
ppm	% Mortality in 24 Hours	
0	0	
500	63	
1000	87	

**Table 11: Death Rates Based on Poison** 

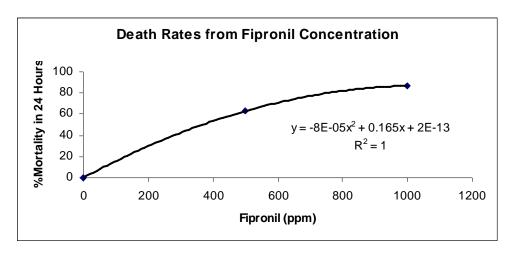


Figure 14: Death Rates Related to Poison

#### Secondary Infected Roaches

Fipronil is a useful poison in that it can spread throughout the colony. Infected roaches can contaminate noninfected roaches through different mechanisms, such as social interactions, dragging the poison with them to the colony, and through cannibalism.

Thus, secondary infection of the roaches can deliver a lethal dosage of the poison, but at a lower concentration and slower death rate. The following equations describe the change in secondary infected roaches in the colony:

$$\frac{dSIM}{dt} = k_{\text{sec}}(NIM) \left( \frac{Infected}{Total} - k_{fipronil,\text{sec}}(SIM) \right)$$

**Equation 19: Change in Secondary Infected Males** 

$$\frac{dSIF}{dt} = k_{\text{sec}}(NIF) \left( \frac{Infected}{TotalRoaches} \right) - k_{fipronil,\text{sec}}(SIF)$$

**Equation 20: Change in Secondary Infected Females** 

$$\frac{dSIB}{dt} = k_{\text{sec}}(NIB) \left(\frac{Infected}{Total} - k_{fipronil,\text{sec}}(SIB)\right)$$

**Equation 21: Change in Secondary Infected Babies** 

Once again, the infection rate is based on the ratio of total infected roaches to the total population. The last term,  $k_{fipronil, sec}$ , describes the death rate of roaches due to secondary infection. Because death rate is proportional to concentration, lower amounts of fipronil will cause lower death rates. When roaches contact an infected roach, it is assumed that the amount transferred is a fraction of the original dosage. However, this dosage will still be lethal.

#### Bait Degradation

As the roaches become attracted to the gel, they will either consume it or carry part of the gel with them. Therefore, the amount of gel will diminish with time. The following equation describes the degradation of bait:

$$\frac{dGel}{dt} = k_{Bait \, consumption} \left( k_{pheromone} NIM + k_{maltose} (NIM + NIF + NIB) \right)$$

**Equation 22: Degradation of Bait** 

The constant, k<sub>bait consumption</sub>, is the rate at which roaches deplete the bait. This value will be larger than the food consumption rate, as larger amounts of gel can stick to the roach. An approximate number for this value is assumed to be about 8mg per roach.

## Completed Model

With the completed model, the user can vary concentrations of each component, the day the poison is added, the total amount of gel matrix, and the variance in food. The user inputs are described below:

Population Model			
Constants			
Maturation rate	0.016666667		
Natural death rate	0.01		
Birth rate	1.142857143		
Roaches eat 'x' grams/day of Food	0.0008		
Roaches contact 'y' grams/day of Bait	0.008		
User Inputs			
Add poison on Day	1000		
Initial Food Supply (grams)	2000		
Add more food every 'x' days	30		
How many grams of food to add?	30		
Maximum Population	20000		
Gel Tube Composition - User Inputs			
Total Gel (grams)	85		
Blatellaquinone (µg)	0.125		
Fipronil (g) [max at .06]	0.06		
Maltose	0		
Carrageenan	84.93999988		

Figure 15: All User Inputs

The following graphs show the various effects of different concentrations in the gel matrix:

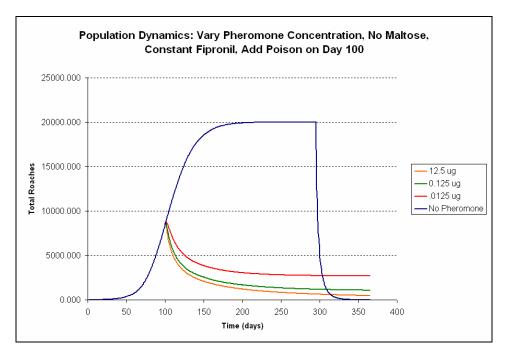
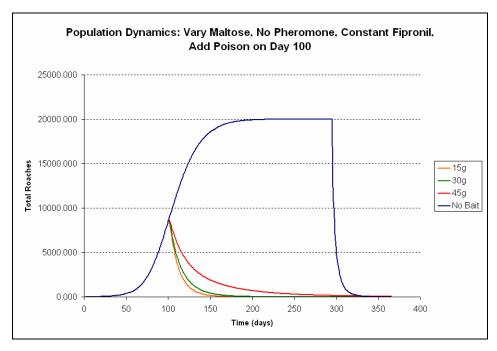


Figure 16: Vary Pheromone



**Figure 17: Vary Maltose Concentration** 

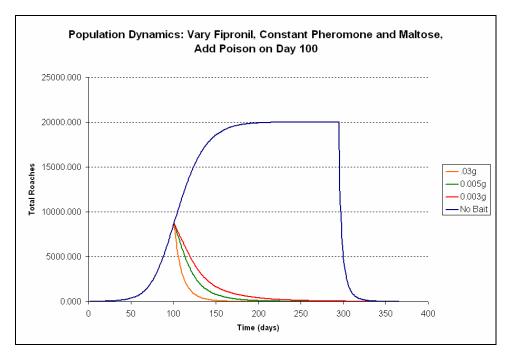


Figure 18: Vary Fipronil

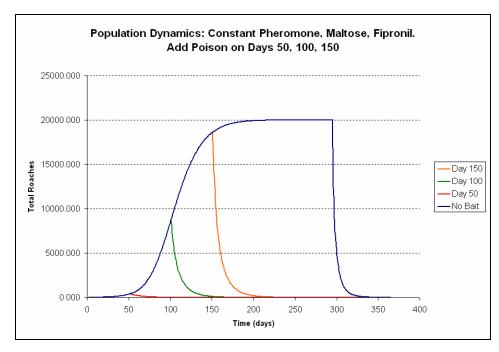


Figure 19: Vary Days

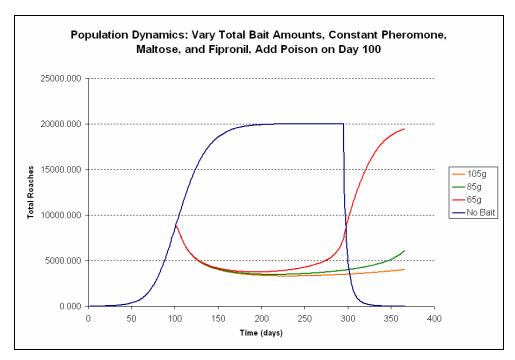


Figure 20: Vary Total Bait

#### Future Work

Several modifications can be made in order to achieve a much more accurate model. While the infection and death rates are based on research articles, the information is still very limited. Actual experiments should be performed with different concentrations of the gel components in order to get more accurate trends. Furthermore, experiments should be performed as to the consumption of the bait. This would allow for more accurate data to describe the depletion of the gel.

#### **DURABILITY AND SPEED REVISITED**

Now that the population model has been explained it becomes easier to explain how durability and speed utilities were found. For both durability and speed there were no trend lines fit to pretty data points. Proceeding in this way, like it was done for toxicity and odor, is impossible because of the 3 parameter dependence. It would also be erroneous to graph them independently of each other and take an average satisfaction value. Because maltose, blattellaquinone, and fipronil are interdependent parameters, and because it is impossible to tell at a glance how varying one will affect speed and durability, an alternate approach was used. This approach is a trial and error procedure in which a large combination of gel compositions are put into the population model. For each composition the effect is examined and related back to a consumer satisfaction percentage based on the performance. Basically you choose a random mixture of maltose, fipronil, and pheromone; put these values into the population model, and see how fast the population dies. This is done systematically for a large number of possibilities. The following is a small part of the table that was created.

Fipronil (mg)	Maltose (g)	Pheromone (μg)		Durability	Speed	Toxicity	Odor	S1 (Ours)	S2 (Maxforce)	β
1 ( 67	(0)	(1.0)	Wi	19%	33%	31%	17%		,	'
10	5	0		0.0%	0.0%	54.2%	84.4%	31.1%	45.0%	1.45
		5		100.0%	14.3%	54.2%	84.4%	54.8%	45.0%	0.82
		10		100.0%	21.4%	54.2%	84.4%	57.2%	45.0%	0.79
		15		100.0%	21.4%	54.2%	84.4%	57.2%	45.0%	0.79
		20		100.0%	21.4%	54.2%	84.4%	57.2%	45.0%	0.79
	15	0		0.0%	0.0%	54.2%	84.4%	31.1%	45.0%	1.45
		5		54.4%	35.7%	54.2%	84.4%	53.3%	45.0%	0.84
		10		70.6%	35.7%	54.2%	84.4%	56.3%	45.0%	0.80
		15		80.6%	35.7%	54.2%	84.4%	58.2%	45.0%	0.77
		20		87.8%	35.7%	54.2%	84.4%	59.6%	45.0%	0.76
	25	0		0.0%	0.0%	54.2%	84.4%	31.1%	45.0%	1.45
		5		17.2%	42.9%	54.2%	84.4%	48.5%	45.0%	0.93
		10		24.4%	42.9%	54.2%	84.4%	49.9%	45.0%	0.90
		15		28.3%	42.9%	54.2%	84.4%	50.7%	45.0%	0.89
		20		30.0%	42.9%	54.2%	84.4%	51.0%	45.0%	0.88
	35	0		0.0%	0.0%	54.2%	84.4%	31.1%	45.0%	1.45
		5		0.0%	42.9%	54.2%	84.4%	45.3%	45.0%	0.99
		10		9.4%	50.0%	54.2%	84.4%	49.4%	45.0%	0.91
		15		11.7%	50.0%	54.2%	84.4%	49.8%	45.0%	0.90
		20		12.8%	50.0%	54.2%	84.4%	50.1%	45.0%	0.90
	45	0		0.0%	0.0%	54.2%	84.4%	31.1%	45.0%	1.45
		5		0.0%	50.0%	54.2%	84.4%	47.6%	45.0%	0.94
		10		0.0%	50.0%	54.2%	84.4%	47.6%	45.0%	0.94
		15		0.0%	50.0%	54.2%	84.4%	47.6%	45.0%	0.94
		20		0.0%	50.0%	54.2%	84.4%	47.6%	45.0%	0.94
	55	0		0.0%	0.0%	54.2%	84.4%	31.1%	45.0%	1.45
		5		0.0%	50.0%	54.2%	84.4%	47.6%	45.0%	0.94
		10		0.0%	50.0%	54.2%	84.4%	47.6%	45.0%	0.94
		15		0.0%	50.0%	54.2%	84.4%	47.6%	45.0%	0.94
		20		0.0%	50.0%	54.2%	84.4%	47.6%	45.0%	0.94

**Table 12: Beta Functions** 

Table 12 only shows values at 10mg of fipronil. The full span of values is 10, 20, 30, 40, 50, and 60mg fipronil. The table does not go beyond 60mg fipronil because it is extremely toxic at this amount.

For every combination of fipronil, maltose, and blattellaquinone, speed and durability satisfaction were found from the population model, toxicity and odor satisfaction from the best fit trend lines, and a  $\beta$  value computed from all of the above. The value highlighted in yellow (0.76) is the minimum beta value.

For durability it is helpful to understand the reason why roaches come back after they are exterminated. The reason that they return is because they were not completely exterminated in the first place. If the consumer sees roaches in their house, the infestation is already extremely bad. Below a certain threshold, the consumer will not see any roaches because roaches prefer to stay hidden and forage for their food in secluded areas. The population model shows several instances where the roach population dips below a certain point and stays below it for months before the population explodes again. This feature of the model allows for reliable durability estimates for a given product composition.

## **β VALUE**

After completing the table using the population model it was desirable to find the smallest  $\beta$  value. This value corresponds to maximum consumer happiness with the new product.

MINIMIZED BETA FUNCTION						
Amount of Fipronil (mg/tube)	10					
Amount of Blattellaquinone (mg/tube)	0.02					
Amount of Maltose (mg/tube)	15000					
S1 (our product)	59.6%					
S2 (Maxforce Gel)	45.0%					
BETA FUNCTION (β)	0.76					

**Table 13: Minimum Beta Value** 

To find  $S_2$  Maxforce was used as the primary competitor. Information from product labels off of their roach bait gel was used to come up with their preference function  $S_2$ . Taking the ratio of these satisfaction values gives a value for beta. This is the actual beta value for our final product. Information on how this particular composition was arrived at is given in the following pricing model section.

#### PRICING MODEL

Once the minimum beta function is found it needs to be related to price and demand so that other options can be explored. The minimum beta function is the best product from the consumer's standpoint. This does not necessarily make it the best product from an economic standpoint.

To assess this, the following economics pricing model is used.

(23) 
$$\Phi(d_1) = p_1 d_1 - \left(\frac{\alpha}{\beta}\right)^{\rho} p_2 \left[\frac{Y - p_1 d_1}{p_2}\right]^{1 - \rho} d_1^{\rho} = 0$$

The equation above gives the relationship between the price of the new product  $p_1$ , the demand of the new product  $d_1$ , the price of Maxforce's product  $p_2$ , and the total amount of revenue, Y, available for this particular market. Y is a constant, and is an estimate of the total amount of money to be made by selling roach bait gels in the southwestern portion of the United States. From the scant data available Y was estimated at \$20,000,000. " $\alpha$ " has to do with the knowledge that consumers have about the new product and can be manipulated through advertisement. " $\alpha$ " was assumed to be 1, which means that consumers are equally aware of the existence of Maxforce's product and the new product. In reality " $\alpha$ " is not 1 because we are a brand new product, but this problem is saved for a later date when advertising is addressed. " $\rho$ " is also assumed to be a constant value of 0.75.

Once all of the constants are accounted for, the demand for the new product at a given price for a given beta value can be found. As indicated above, to be valid, the equation must always equal 0. Thus it can be seen what kind of price-demand relationships are allowed for a given value of beta. This is the equation that finally connects changes in product composition to changes in FCI, TCI, and consequently NPV. A change in composition changes the beta value; which subsequently alters the allowable price demand relationships. This in turn dictates how many units we can expect to sell, and for how much per year.

To find the optimal product composition different values of beta must be selected. For each of these beta values the price should be varied across an acceptable range. A table is created that shows the demand for different product prices and different beta values. The following table shows only beta at 0.8, but beta values of 0.76, 0.86, 0.90, and 0.95 were also explored.

$P_1D_1$	P₁ (\$/unit)	D <sub>1</sub> (# of units)	α	β	ρ	P <sub>2</sub> (\$/unit)	Υ	_	Φ	NPV (millions)
16451747.57	5	3290349.513	1	0.80	0.75	6.67	20000000		0.000	88.0
14569945.96	6	2428324.327	1	0.80	0.75	6.67	20000000		0.000	89.7
12564267.55	7	1794895.364	1	0.80	0.75	6.67	2000000		0.000	75.2
10619035.5	8	1327379.437	1	0.80	0.75	6.67	20000000		0.000	59.9
8858085.114	9	984231.6794	1	0.80	0.75	6.67	20000000		0.000	45.3
7338343.835	10	733834.3835	1	0.80	0.75	6.67	20000000		0.000	32.3
6067001.241	11	551545.5673	1	0.80	0.75	6.67	20000000		0.000	21.1
5023220.465	12	418601.7055	1	0.80	0.75	6.67	20000000		0.000	11.9
4174731.669	13	321133.2053	1	0.80	0.75	6.67	2000000		0.000	4.2
3487646.181	14	249117.5844	1	0.80	0.75	6.67	20000000		0.000	-2.0
2931149.894	15	195409.993	1	0.80	0.75	6.67	20000000		0.000	-7.1
2479149.8	16	154946.8625	1	0.80	0.75	6.67	20000000		0.000	-11.2
2110385.346	17	124140.3145	1	0.80	0.75	6.67	20000000		0.000	-14.7
1807894.151	18	100438.5639	1	0.80	0.75	6.67	20000000		0.000	-17.5
1558288.818	19	82015.20092	1	0.80	0.75	6.67	20000000		0.000	-19.8
1351051.498	20	67552.57492	1	0.80	0.75	6.67	20000000		0.000	-21.8
1177923.767	21	56091.60795	1	0.80	0.75	6.67	20000000		0.000	-23.4
1032408.758	22	46927.67083	1	0.80	0.75	6.67	20000000		0.000	-24.8
909377.3362	23	39538.14505	1	0.80	0.75	6.67	20000000		0.000	-25.9
804761.7432	24	33531.7393	1	0.80	0.75	6.67	20000000		0.000	-26.9
715319.3388	25	28612.77355	1	0.80	0.75	6.67	20000000		0.000	-27.8
638451.0355	26	24555.80906	1	0.80	0.75	6.67	20000000		0.000	-28.5
572061.8171	27	21187.47471	1	0.80	0.75	6.67	20000000		0.000	-29.1
0	28	0	1	0.80	0.75	6.67	20000000		0.000	-34.7
0	29	0	1	0.80	0.75	6.67	20000000		0.000	-34.7
0	30	0	1	0.80	0.75	6.67	20000000		0.000	-34.7

Table 14: NPV versus price at 0.8 Beta

Another facet of the beta function was dealing with more than one beta function of the same value. For example, for a beta function of 0.86 in order to get an NPV number

component amounts have to be specified. So what happens if more than one set of components yields the same beta value? To remedy this problem each set of components with the same beta value was put into another table. From this table the reactant cost for each set of components was calculated. Then the set of components with the minimum associated cost was chosen to go into the NPV calculations.

β	Fipronil (mg)	Maltose (g)	Pheromone (µg)	Reactant Cost
0.86	20	15	5	93,369
0.86	30	5	5	95,169
0.86	30	5	10	95,185
0.86	30	15	10	95,185
0.86	40	5	10	96,986
0.86	40	5	15	97,002
0.86	40	5	20	97,018
0.9	10	25	10	88531
0.9	10	35	15	88547
0.9	10	35	20	88562
0.9	20	25	15	90287
0.9	20	25	20	90293
0.9	30	15	5	91995
0.9	40	5	5	93735
0.9	50	15	20	95522

**Table 15: Duplicate Beta Functions** 

Using the pricing model to vary beta and potential selling prices several curves are obtained that relate price of a given product to the NPV over a ten year period.

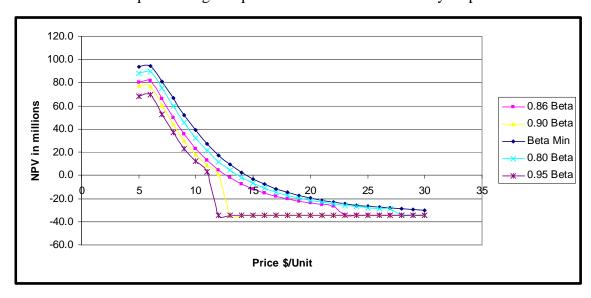


Figure 21: NPV vs Price for different Betas

Graphical analysis of these results yields the necessary information. The composition of the product is the composition that gives the minimum beta value and the product should be sold at \$6.00 to yield the maximum amount of profit. This price has an associated demand of roughly 2.5 million and would yield an NPV of just under 100 million after 10 years. The following table shows the composition of our product again.

MINIMIZED BETA FUNCTION						
Amount of Fipronil (mg/tube)	10					
Amount of Blattellaquinone (mg/tube)	0.02					
Amount of Maltose (mg/tube)	15000					
S1 (our product)	59.6%					
S2 (Maxforce Gel)	45.0%					
BETA FUNCTION (β)	0.76					

**Table 16: Product Composition** 

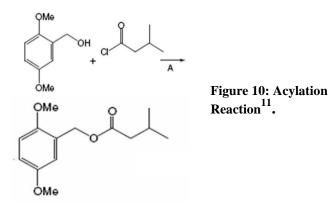
At first glance it would appear odd that the composition of our product is the best economically for us and for our consumers. But it is important to remember that in many instances smaller values of the critical reactants were more effective at combating roach infestations. For instance, too much pheromone actually disorients roaches and drives them away instead of attracting them. So a careful amount of blattellaquinone must be applied to be maximally effective. Also, based on the population model it is not always good to have lots of maltose either. This is because too much maltose causes the roaches to consume the bait faster which causes it to run out faster. So in many cases if the roaches consume it at a slower rate because they are less attracted to it, bait degredation does not become a factor and the poison has a greater chance to spread through the population.

# PLANT/PROCESS DESIGN

Blattellaquinone is not available for purchase. Therefore, synthesis of this compound must be included in the process design. This process is based off of the blattellaquinone

research from Cornell University<sup>11</sup>. The laboratory synthesis provides the necessary reactants and methods needed to develop the process plant.

Synthesis of blattellaquinone is possible through two reactions. First, acylation is performed by adding isovaleryl chloride to 2, 5 dithmethoxybenzyl alcohol, yielding an intermediate ester and HCl<sup>11</sup>.



This reaction takes place in a solution containing DMAP (dimethylaminopyridine), pyridine, and dichloromethane <sup>11</sup>. Both DMAP and pyridine act as nucleophilic catalysts in the acylation reaction, while dichloromethane is the organic solvent. Following acylation, liquid-liquid extraction is used with diethyl ether to remove the ester from the mixture <sup>11</sup>. To isolate the ester compound completely, diethyl ether is removed with an evaporator <sup>11</sup>. Because ether has a low boiling point of approximately 34.6°C, not much heat is needed to vaporize the solvent.

The second reaction is oxidation<sup>11</sup>. The intermediate ester is mixed with acetonitrile in the presence of cerium ammonium nitrate, oxidizing the ester<sup>11</sup>. Cerium ammonium nitrate acts as a catalyst for the reaction.

The result of this reaction is the desired product, blattellaquinone. The compound must be extracted out of the reactant mixture using dichloromethane<sup>11</sup>. Once again, evaporation is used to remove the solvent and isolate the pheromone<sup>11</sup>.

With the pheromone synthesized, it is then ready to be mixed with the other product ingredients. Carrageenan must be heated prior to mixing to ensure its liquid form. It takes a temperature of approximately 50°C to melt the compound<sup>16</sup>. When mixed with the other ingredients, the carrageenan will cool, forming a gel. The gel product is then ready to be pumped to a packager for distribution.

This overall process was used to generate the following PFD's for the plant:

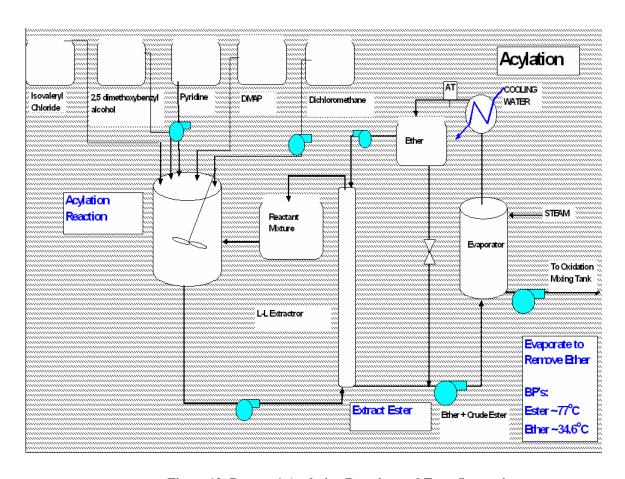


Figure 12: Process 1-Acylation Reaction and Ester Separation

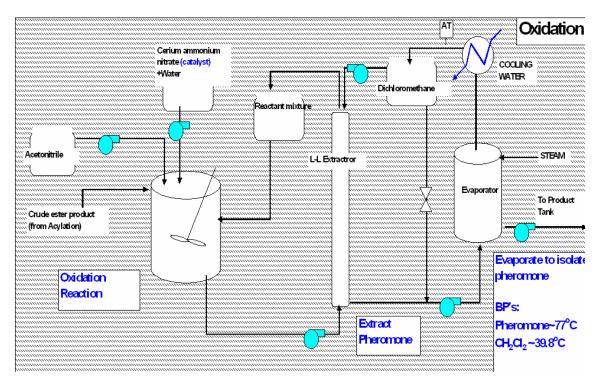


Figure 13: Process 2- Oxidation Reaction and Blattellaquinone Separation

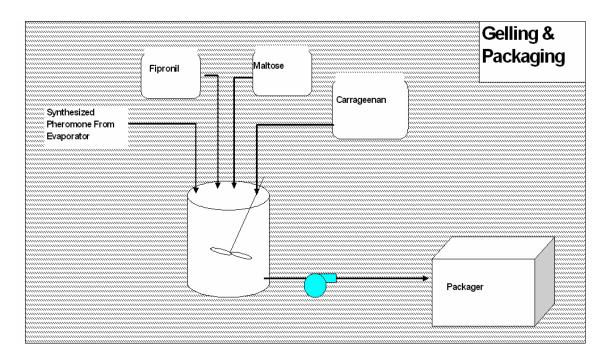


Figure 14: Process 3 – Product Mixer and Packaging

# **Equipment Design and Purchased Costs**

## **REACTANTS**

Sizing of the process equipment is dependent upon the amount of blattellaquinone required per year. This amount is determined by the composition of each gel tube and the number of units to be produced. These parameters are resolved through the utility functions and demand model.

The final amount of blattellaquinone yielded from the lab synthesis is proportional to the amount of a given reactant. This ratio, multiplied by the amount of pheromone needed on a large scale, gives the amount of reactant needed for the plant. The following equation was used to scale up the reactants:

$$\text{Reactant}_{\text{LargeScale}} = Pheromone_{\text{LargeScale}} \times \frac{\text{Reactant}_{\text{Experiment}}}{Pheromone_{\text{Experiment}}}$$

Equation 23: Equation for Reactant Scale Up

The amount of reactants needed for the process, multiplied by the prices for each reactant, gives the cost of raw materials. Prices for all reactants and gel ingredients are listed below <sup>15</sup>.

Listed Prices							
Reactant / Ingredient	\$/g	\$/mL					
Isovaleryl Chloride	0.310	n/a					
2,5-Dimethoxybenzyl Alcohol	3.13	n/a					
Pyridine	0.0749	0.073					
4-Dimethylaminopyridine	0.887	n/a					
Dichloromethane	n/a	0.019					
Cerium Ammonium Nitrate	0.550	1.370					
Acetonitrile	n/a	0.049					
Ether	n/a	0.017					
Fipronil	1.45	n/a					
Maltose	0.0450	n/a					
Carrageenan	0.00830	n/a					

Figure 22: List Prices for Reactants & Ingredients<sup>15</sup>

#### **TANKS**

All storage tanks in the plant are designed to hold one month's supply of reactants. For safety reasons, this capacity is increased by 1.5 times. To avoid corrosion, all tanks are to be constructed from 304 stainless steel. Using available correlations, the prices for each tank can be obtained<sup>12</sup>.

## LIQUID-LIQUID EXTRACTORS

The scale up of extractors is based upon the amount of stages needed to achieve an efficient extraction. It was assumed that at least 10 stages are needed to effectively remove the intermediate ester and blattellaquinone from their respective reactant

mixtures. Mechanical agitation, or a Scheibel extractor, was chosen because it allows good contact between the solvent and the mixture. From here, the equivalent height of a theoretical stage can be read directly from given tables<sup>12</sup>. This gives the height of the extractor by the following equation<sup>14</sup>:

$$HETS = \frac{Column \; Height}{\# Stages}$$
 Equation 24: Determining Extractor Height

Extractor prices can be approximated by using the correlations for distillation columns<sup>12</sup>.

#### **EVAPORATORS**

To prevent damage to the intermediate ester and blattellaquinone, evaporators are chosen to remove the solvent. Evaporators are useful when heat sensitive components are involved 12. The design is based on the heat transfer area needed to evaporate the solvent. It is assumed that when the solvent fills the evaporator, it takes the form of a cylinder. Thus, the equations for the volume and surface area of a cylinder can be used. By assuming that the length of the cylinder is equal to six-times the radius, it is possible to solve for surface area based on volume. Changing the ratio of length to radius is an optimization parameter that affects vapor velocity and convection. The following equation gives the heat transfer area of the evaporator based on the volume of the solvent:

$$SA = 12\pi \left(\frac{V_{Solvent}}{6\pi}\right)^{2/3}$$
 Equation 25: Heat Transfer Area of Evaporator

The heat required to vaporize the solvent is provided by steam. To calculate the amount of steam needed, a heat balance is performed.

Qheat solvent= 
$$mCp(\Delta T)$$
  
Qvaporize solvent =  $m(\Delta H)$ 

This total heat is then used to calculate the mass of steam required.

47

## QTotal= $mCp(\Delta T)$ Steam

#### **MIXING TANKS**

Because kinetic data are not available, mixing tanks are chosen to perform the reactions. The reactants consist of both powdery solids and liquids. Thus, ribbon blenders are selected, as they can mix both solids and liquids effectively<sup>12</sup>. Sizing of these mixers are based on the sum of all reaction components needed for one month's capacity.

The final mixer must be designed to mix all ingredients within the gel matrix. Because the gel media is assumed to be a very high viscosity, a kneader mixer must be used<sup>12</sup>.

Purchased costs for each mixer are determined by the available correlations <sup>12</sup>.

#### **PACKAGER**

Before the gel can be distributed, it must be packaged in plastic tubes. One type of packager capable of performing this function is a HORIX 32 carousel filling unit<sup>9</sup>. Designed to handle gels, these filling units can continuously package the product without disrupting the overall process.

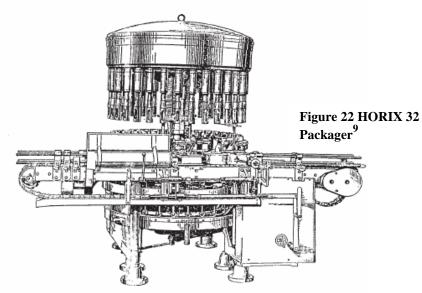


FIG. 21-45 HORIX 32 station carousel-type liquid filler for glass and plastic bottles and metal cans

#### **PUMPS**

The majority of all fluids that require pumping are of low viscosity. Thus, centrifugal pumps are the logical choice for fluid flow. To prevent corrosion, these pumps will be constructed from 316 stainless steel. Applying the correlations provided, the purchased cost can be obtained <sup>12</sup>.

To transport the gel product from the final mixing tank, a pump that can handle high viscosities is required. This can be achieved with a positive displacement pump.

Assuming that the pump is made of stainless-steel, given correlations can once again be used to determine purchased costs<sup>12</sup>.

The power requirements for each pump can be calculated with the following equation<sup>3</sup>:

$$Horsepower = \frac{(GPM)(\Delta P)}{(1715)(Efficiency)}$$
 Equation 26

In order to use this equation, both pressure drop and efficiency are assumed to be 20 psi and 80%, respectively. By specifying the amount of batches per day, the number of batches per second is determined. It is assumed that each step in the process (acylation, oxidation, packaging) is one-third of the total batch time. In the acylation and oxidation processes, it is further assumed that loading of the reactants and the fluid transfer from the extractor is 20% of the process, while the extraction and evaporation processes are 80%. Flowrates for these pumps can then be calculated per batch, as well as their respective power requirements and electrical costs.

#### FIXED/TOTAL CAPITAL COSTS

Both the fixed and total capital investments are estimated as the percentage of the delivered-equipment cost  $^{12}$ . This total equipment cost is obtained from the sum of the costs of all designed equipment. Using this method, the FCI and TCI for this plant are determined to be \$1.4 million and \$1.6 million, respectively. While an approximation, the accuracy of this method has been shown to be within  $\pm 10\%^{12}$ .

#### PRODUCTION COSTS

Estimation of the annual cost to produce the bait product is dependent on several factors. First, the cost of raw materials is calculated on an annual basis. Next, operating labor can be approximated based on plant capacity<sup>12</sup>. With this method, at least 40 employee hours per day per processing step are needed. Using labor information, an hourly wage of \$22.03 is obtained<sup>17</sup>. Finally, utilities for the process can be determined by calculating the annual cost of steam, cooling water, and electricity required. It is assumed that the plant is in operation for 350 days a year, with at least 15 days set aside for routine maintenance and sterilization of the maltose tank. This results in an annual production cost of \$17.4 million.

## PLANT LOCATION AND TRANSPORTATION COSTS

In order to effectively distribute the bait product throughout the Southwest region, a plant location was decided based on equidistant travel to all locations. Located around the center, Farmington, NM, is an acceptable location for the plant. With a population of about 41,000, there will be enough manpower to run the facility.

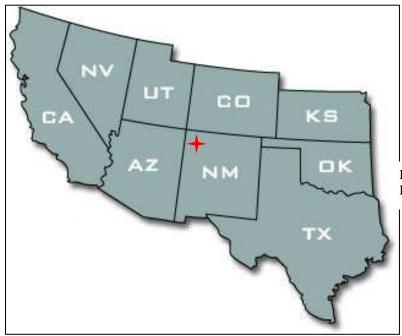


Figure 23: Plant Location – Farmington, New Mexico<sup>20</sup>

The costs for transportation are assumed to be 10% of the raw material cost. This accounts for the delivery of the product to all distribution centers.

## **ECONOMIC ANALYSIS**

The revenue generated from the process is calculated by multiplying the units sold per year by the cost of each unit. At \$6 a unit for 2.5 million units, the revenue per year is around \$15 million. Assuming no variance in reactant or utility costs and a 10 year plant life, the sum of the cash flows gives the approximate NPW. For 10 years, the NPW is found to be \$90 million. With an NPW greater than zero, this is a profitable process.

## **ENVIRONMENTAL CONCERNS**

Many of the reactants are quite harmful to the environment. Acetonitrile can weakly adsorb to soil, while pyridine can adsorb to clay<sup>7</sup>. If released into the water, fipronil, methylene chloride, and acetonitrile can be deadly to aquatic life, especially fish<sup>7</sup>. If released in the air, both pyridine and methylene chloride can last for a while before

degradation. Pyridine can last for over 30 days in the air, while methylene chloride can take up to several months before it is decomposed<sup>7</sup>.

# **CONCLUSION**

The findings of this project conclude that a new gel bait design based on blattellaquinone can be a profitable venture. After applying the utility functions, it is determined that the final composition of the gel will consist of 20ug/tube blattellaquinone, 0.01g/tube fipronil, 15g/tube maltose, and 50g/tube carrageenan. The pricing model, used in conjunction with the process/plant cost analysis, requires that 2.5 million units of the gel be sold a year, with each unit costing \$6. This results in a net present value of about \$90 million for ten years, indicating a very profitable process.

### **FUTURE WORK**

There are a couple ways to optimize the process for future designs. First, both catalysts (cerium ammonium nitrate and DMAP) are very expensive, contributing to almost half of the cost of raw materials. By performing in-depth experiments on the chemistry of these catalysts, it may be possible to regenerate each compound, dramatically reducing costs. Secondly, costs can be reduced by reusing the reactant mixture. Recycling the reactant mixture to the reaction tank can allow for unreacted compounds to go to completion, reducing the amounts of initial reactants needed.

More research should be done on the nature of the constants found for the population model. There was scant information available for the degree of attraction of roaches to maltose. Also, the differences in the metabolisms of nymphs and adults was not taken into account, but could be incorporated with additional research. Average amounts of edible food per household, average household roach infestations, and average roach ingestion rates should also be verified.

The approximations<sup>12</sup> used for the capital and production costs are not entirely accurate. Many of the values are based off of percentages from average data of other plants.

Furthermore, the pricing of some equipment falls below the minimum cost in the given trends. In this case, the lowest equipment price on the chart was chosen. This contributes to the calculated NPW and the associated costs having a significant degree of error.

In addition to the aforementioned issues, the pricing model should be extended and explored in more depth. This report contains no assessment of factors such as: risk, uncertainty, variance in reactant costs, and inflation. It also does not rectify the assumptions inherent in the population model itself; namely assuming that the consumer will have equal knowledge of both products.

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