Insect Repellent Design

Final Report

Erin Ashley

Scott Doman

May 4, 2006

Introduction
The Repellent Market

- DEET (N,N-diethyl-m-toluamide) was discovered in 1946
- The market has remained largely unchanged since then
- Consumer pressures have led companies to seek gentler and safer alternatives to DEET
- OFF! and Cutter are the major players in the repellent market

Introduction
The Repellent Market

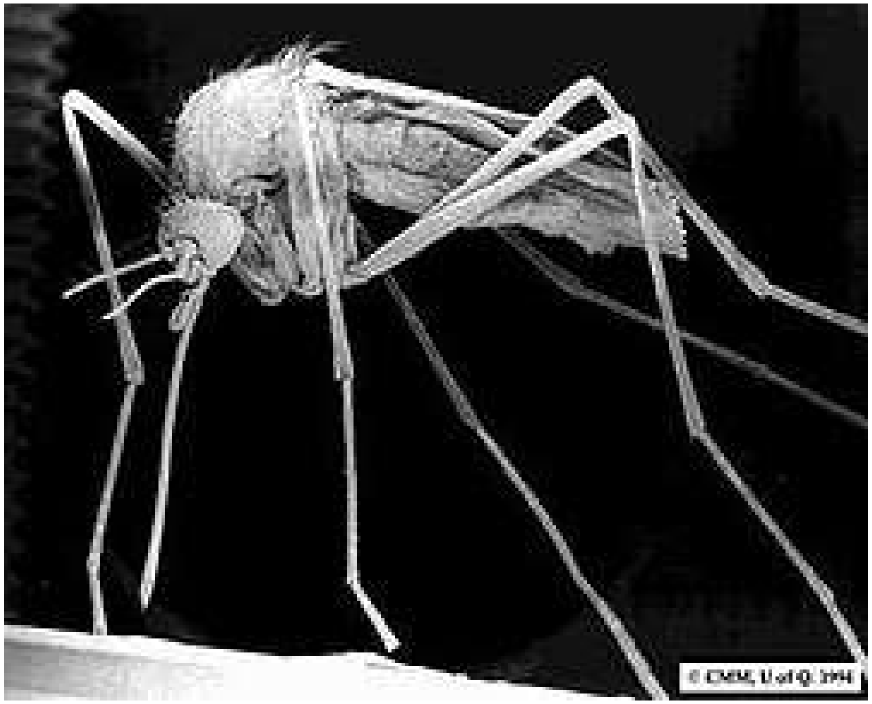
- The company that can come up with an economically feasible, user-friendly, safe product stands to gain a large share of the market.

- Initial aim: develop a new repellent that will accomplish these objectives
  - Investigate insect/repellent interactions

Background
Insect Receptors

Types of Receptors

- Thermoreceptors
- Mechanoreceptors
  - Tactile receptors
  - Sound receptors
- Photoreceptors
- Chemoreceptors
  - Gustatory receptors
  - Olfactory receptors



Source: http://www.mediabum.com/images/mosquito.jpg

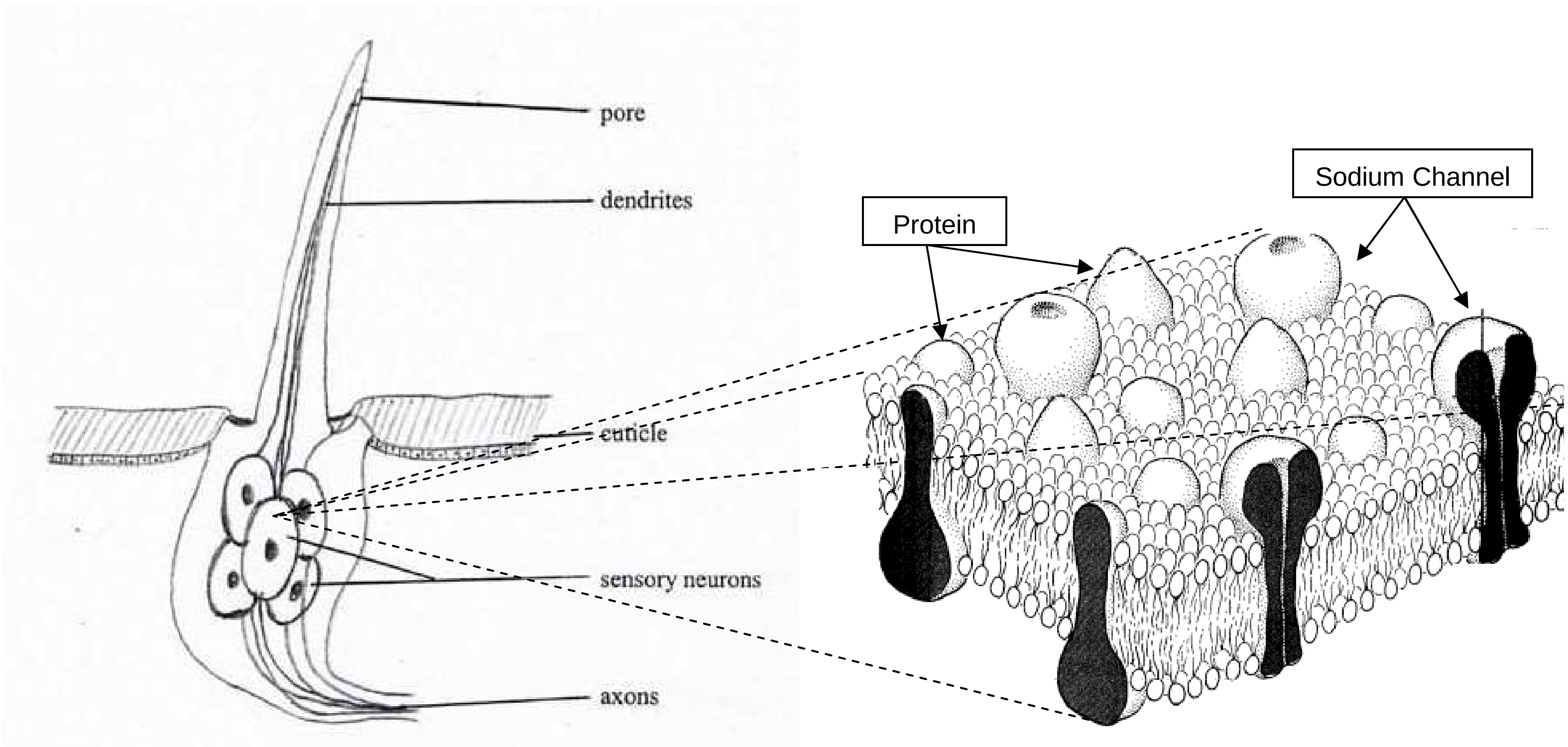
Background

Insect Chemoreceptors

- Olfactory chemoreceptors are usually located on the antennae
- Each antenna is covered in hair-like sensilla containing neurons
- Each antenna can have as many as 75,000 receptor cells

Source: http://www.insectscience.org/3.2/ref/fig5.jpg

Background
Chemoreceptor Mechanism



Source: http://www.bioweb.uncc.edu/BIOL3235

Source: http://www.pneuro.com/publications/insidetheneuron

Background

Insects of Interest

- How do insects use their receptors to find humans?
  - Visual Stimuli: long distances
  - Chemical Stimuli: short distances
    - Carbon dioxide from skin and breath
    - Lactic acid from skin
  - Temperature Stimuli: very close range

- What types of insects are interested in humans?
  - Mosquitoes
  - Ticks
  - Fleas

Source: http://static.howstuffworks.com/gif/mosquito6a.jpg

Background

Repellent Mechanisms

- What we need to know
  - How insect repellents work
    - “Blockers”-blinds the insect to the presence of its meal
    - “Repellents”-works opposite of an attractant
    - “Alarms”-sends a danger signal to the insect’s brain
  - Characteristics of a certain molecule that give it repellent properties

Background

Repellent Mechanisms

- Unfortunately, the true mechanisms of repellents are not known!
- According to Dr. Joel Coats at Iowa State University, "Structure-activity relationships of repellents are unclear, and little definitive work has been done….Vapor pressure is the only parameter significantly related to mosquito repellent activity."

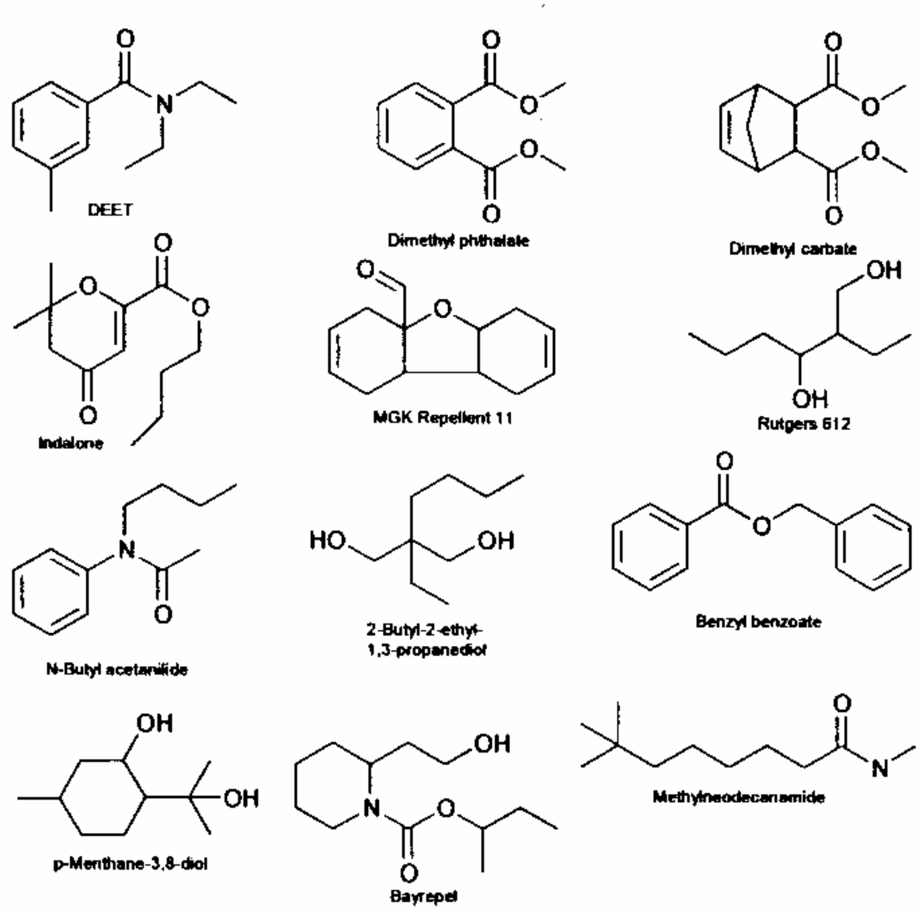


Figure 1. **Structures of several insect repellents.**

Source: Coats, Joel, "Insect Repellents- Past, Present, and Future"

Background

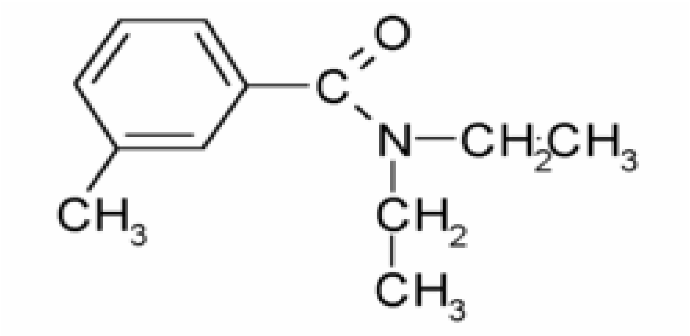
A New Pursuit

- Instead of developing a new repellent, we plan to re-engineer an existing repellent
- Market research is performed to determine which repellents to re-engineer

Background

Repellents in the U.S. Market

- DEET
  - The most commonly used insect repellent
  - One of few repellents that can be applied to the skin
  - Unpleasant scent
  - Damages plastic and other synthetic materials

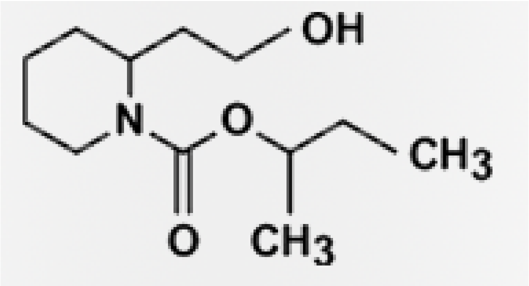


Source: http://en.wikipedia.org/wiki/DEET

Background

Repellents in the U.S. Market

- Picaridin
  - Recently introduced in the US in Cutter Advanced
  - Shown to be as effective as DEET at equal concentrations
  - Recommended by Center for Disease Control (CDC) and World Health Organization (WHO)
  - No scent
  - Does not damage synthetic materials



Source: http://picaridin.com/science.htm

Background

Repellents in the U.S. Market

- Cutter Advanced contains Picaridin at 7% concentration
- DEET is offered at concentrations up to 100%
- There is room in the market for more Picaridin products

Cutter Advanced: 7% Picaridin

Deep Woods OFF! For Sportsmen: 100% DEET

Achieving the Objective

- Develop a new repellent formula with Picaridin as the active ingredient
  - Create a utility function to measure the wants and needs of repellent consumers
  - Design a production and distribution model
  - Analyze the economics and maximize the profit of this formula

Caveats

- This is a preliminary model
- Many assumptions made based on educated guesses

The Utility Function

- Describes the satisfaction a consumer receives from using a product:

$$U = \Sigma U_i w_i$$

U is the utility; w is the weighted average of each characteristic of the product that the consumer deems important; i is each characteristic

- Need to decide w, construct equations for each characteristic

The Utility Function
Repellent Characteristics

- Maximize utility of each of the following characteristics for an overall maximum utility
  - Effectiveness
  - Durability
  - Feel
  - Form (Lotion or Spray)
  - Toxicity
  - Scent

The Utility Function

Weights

- A sample population was surveyed to determine the preferences of consumers.
- Target consumer: campers and hikers
- These preferences were used to assign w_i to each physical property (sum= 1).
- Assumptions

Property	Weight
Effectiveness	0.29
Durability	0.24
Feel	0.19
Form	0.14
Toxicity	0.09
Scent	0.05

The Utility Function

Ingredients

- Each ingredient chosen to increase the overall utility
  - To increase effectiveness and durability: *use Picaridin*
  - To improve scent and texture, *add fragrance and aloe*
  - To dissolve ingredients and lower cost, *add ethanol*

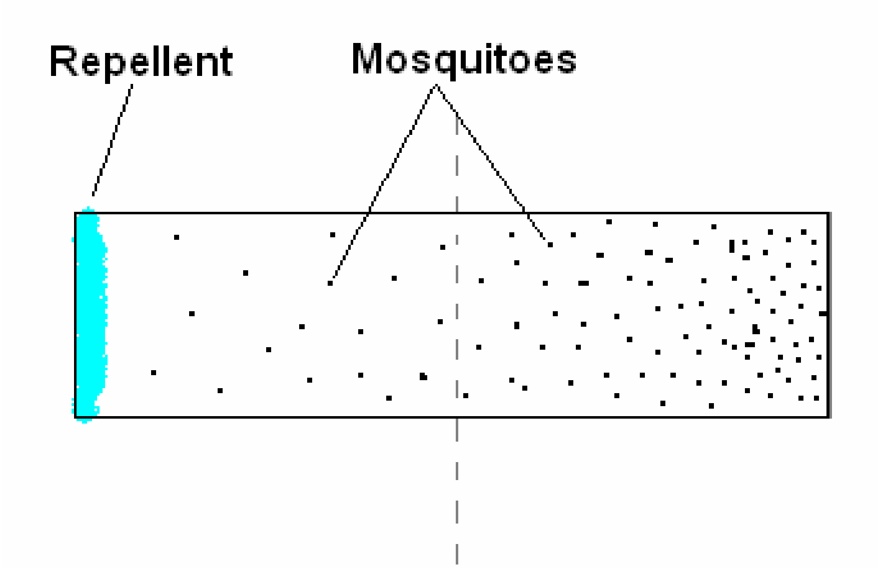
The Utility Function

General Method

- For each chosen characteristic:
  1. Relate utility to levels of the characteristic
  2. Relate these levels to results of a consumer test
  3. Relate test results to some physical property of the repellent formula
  4. **Relate utility to repellent physical property for optimization**

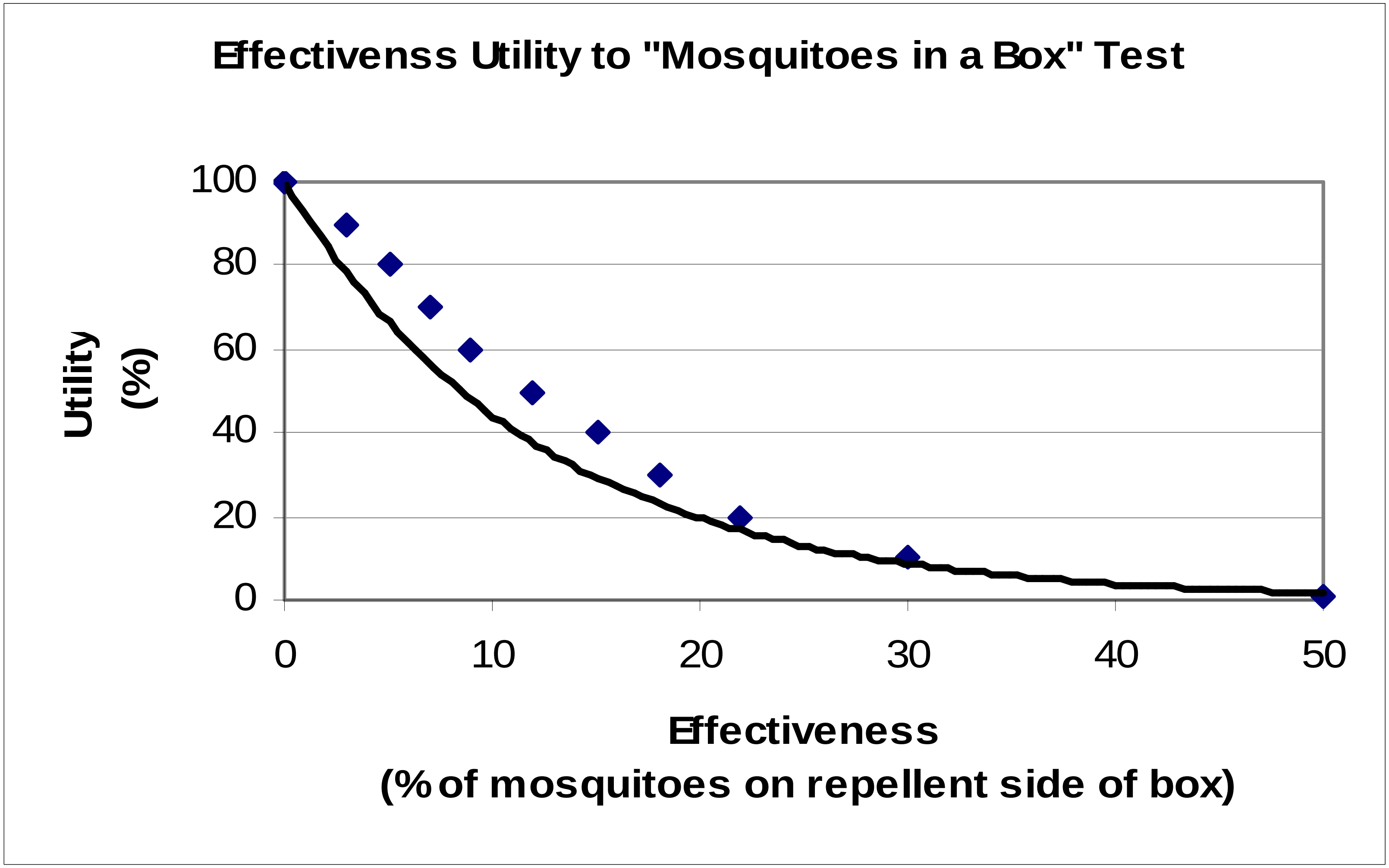
The Utility Function
Effectiveness

- Industry Standard Test
  - Mosquitoes in a box with a repellent sample on one side
  - Percentage of the population on that side of the box after a certain time shows the repellent's effectiveness.



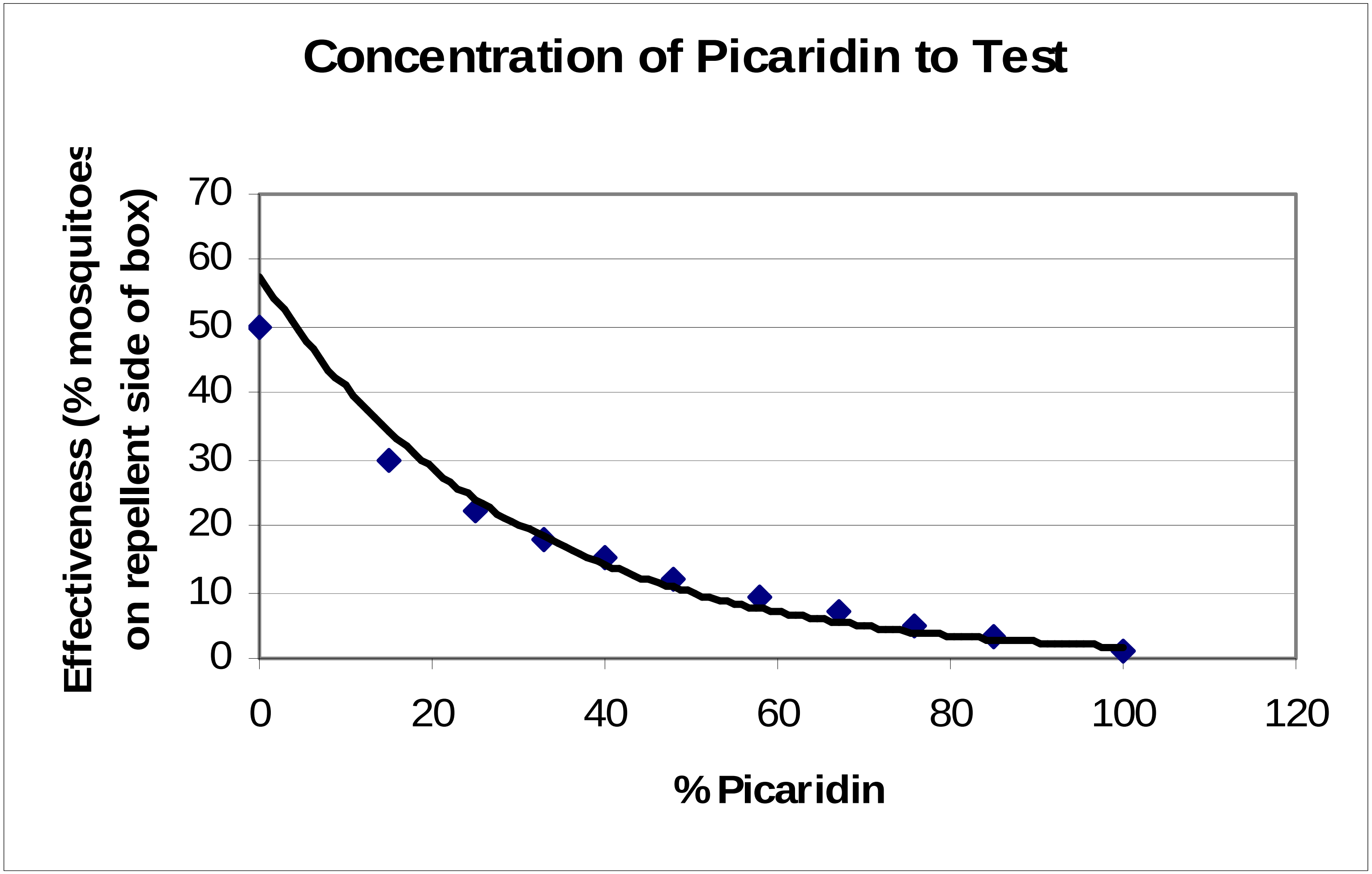
The Utility Function

Effectiveness



The Utility Function

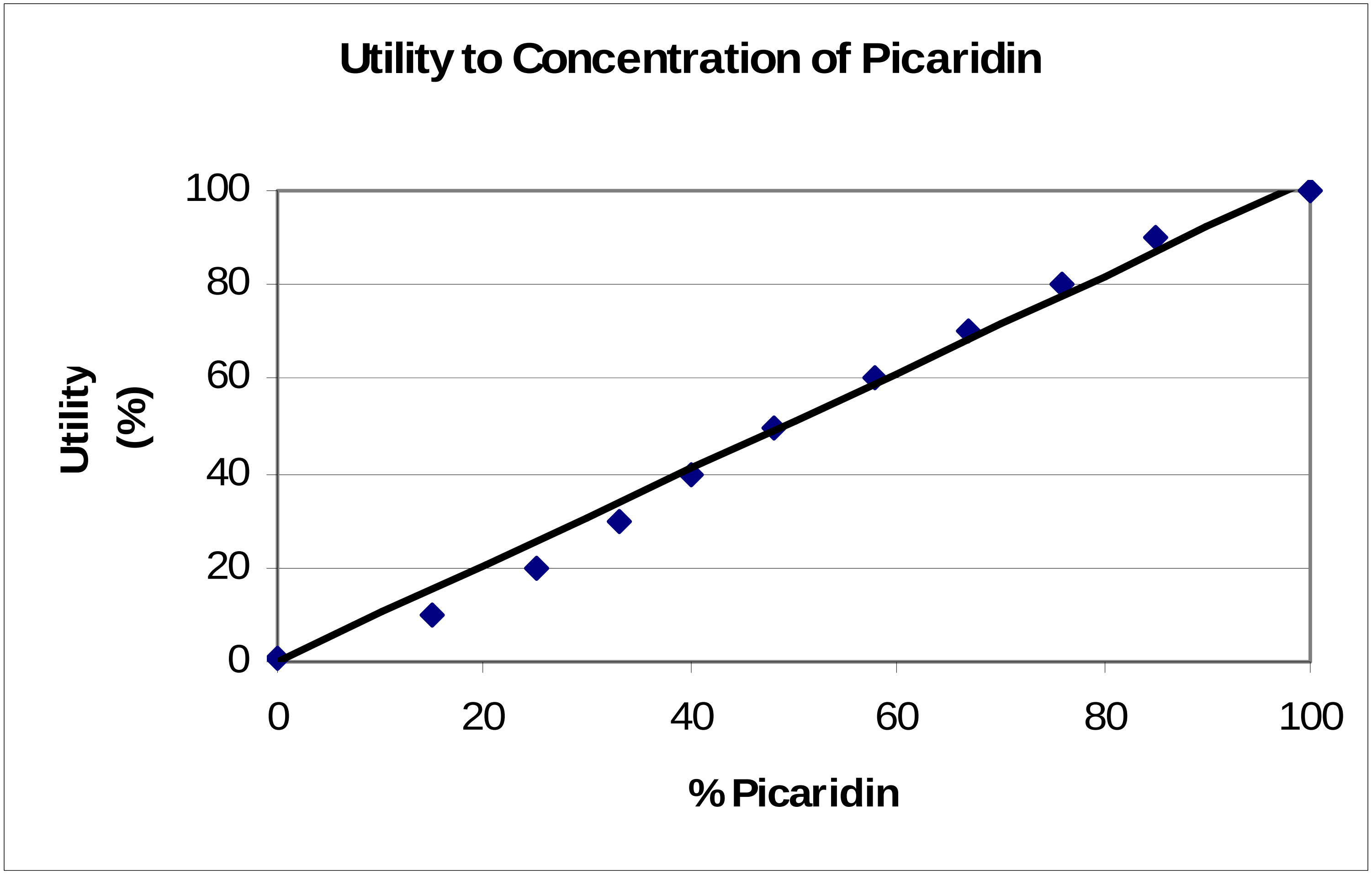
Effectiveness



The Utility Function

Effectiveness

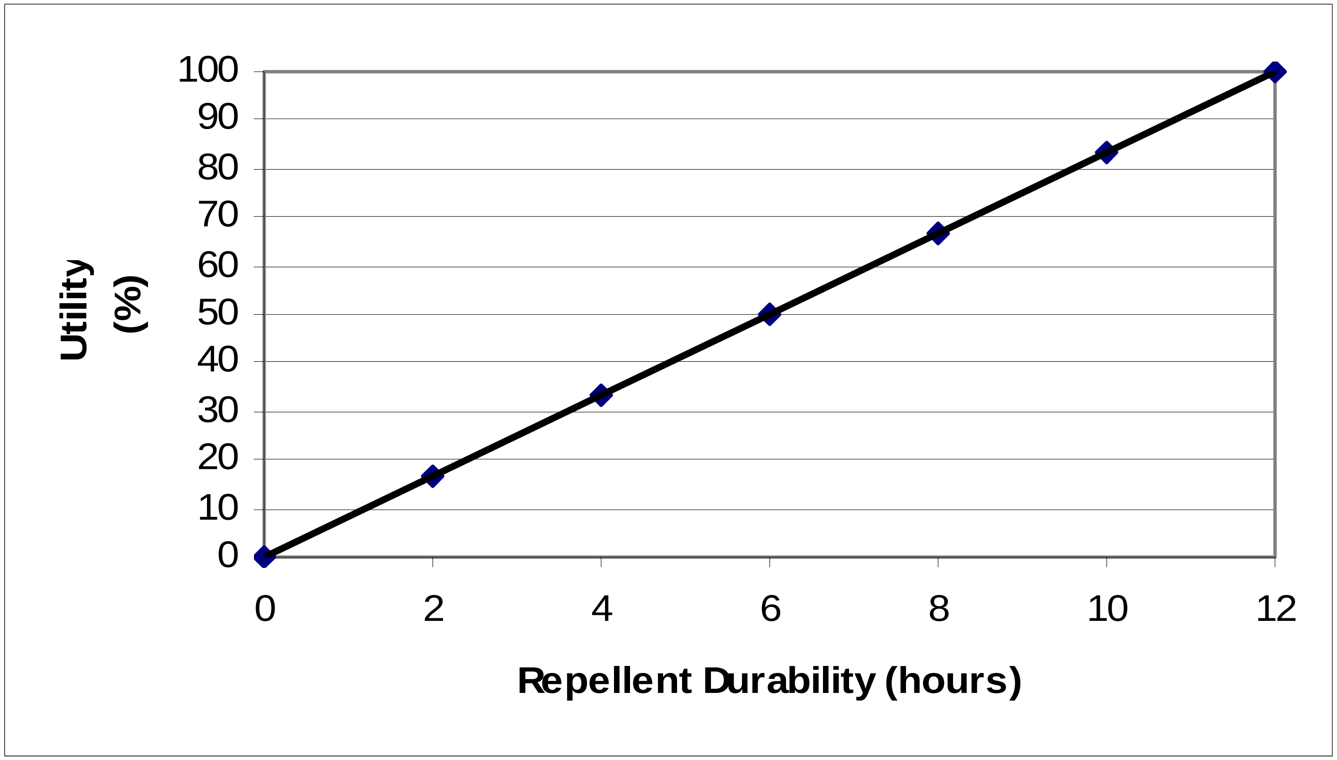
Final Utility to Picaridin Relationship:
U = 1.023*%Picaridin



The Utility Function

Durability

- Relate durability utility to levels of durability: *Amount of time repellent stays effective*



The Utility Function

Durability

- Relate time to physical property of formula: *Vapor pressure of the mixture*
  - Model evaporation of repellent off skin as a function of time
  - Calculate the amount of time needed for the concentration of repellent at a certain distance from the skin to fall below a set threshold concentration

The Utility Function

Durability

- Fick's second law of diffusion

$$\frac{\partial c_A}{\partial t} = D_{AB} \frac{\partial^2 c_A}{\partial z^2}$$

  - c_A = concentration of component A
  - D_{AB} = diffusion coefficient of component A
  - t = time
  - z = distance from skin, set at 0.3 m

The Utility Function
Durability

- Fick's second law becomes

$$\frac{\partial c_A}{\partial t} = \frac{c_{As} \cdot e^{\frac{-z}{2\sqrt{D_{AB}t}}}}{4t\sqrt{\pi}}$$

where C_{As} = surface concentration

$$c_{As} = \frac{p_A}{RT} = \frac{x_A(VP)}{RT}$$

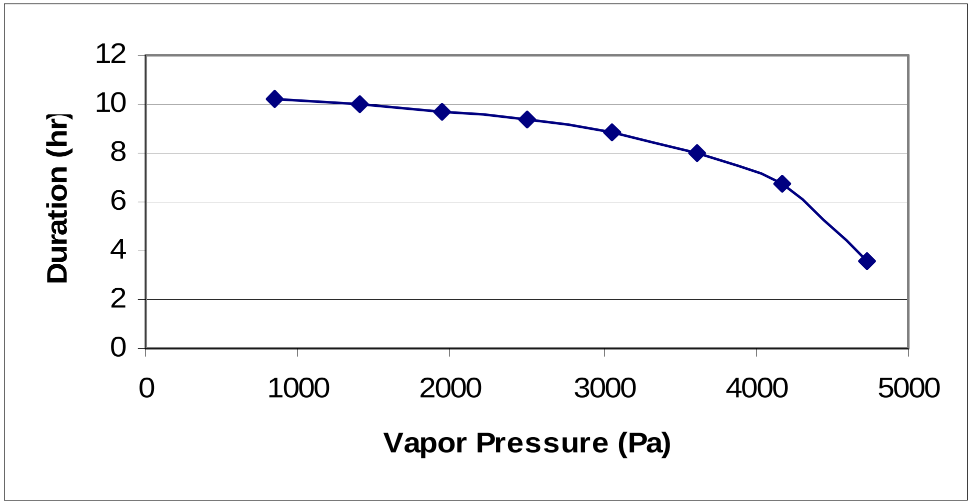
using Raoult's Law approximation

The Utility Function

Durability

- Set time interval = 10 minutes
- Set initial concentrations of all components
- Start: C_{As} = partial pressure of each component
- Calculate C_A of each component at z = 0.3 m
- Calculate amount of moles lost from liquid
- Recalculate liquid concentrations
- Recalculate new C_{As} based on new concentrations
- Repeat process until C_A of Picaridin reaches 0.05 mol/m^3

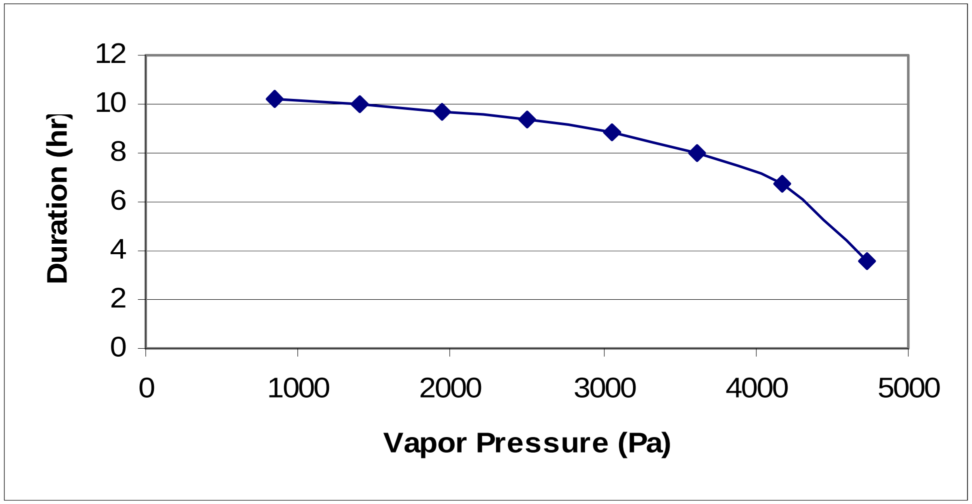
The Utility Function
Durability

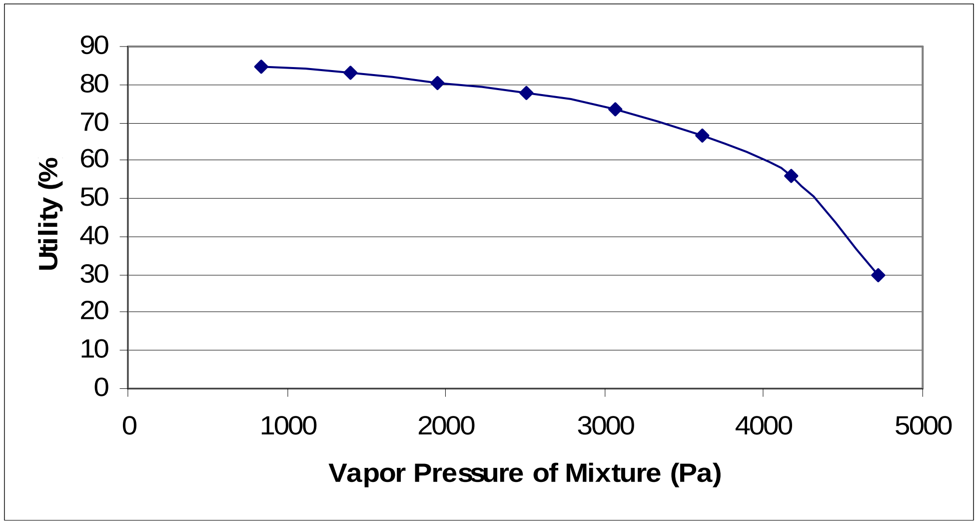


After correlating durability to several physical properties, initial vapor pressure of the mixture showed the strongest relationship.

The Utility Function

Durability





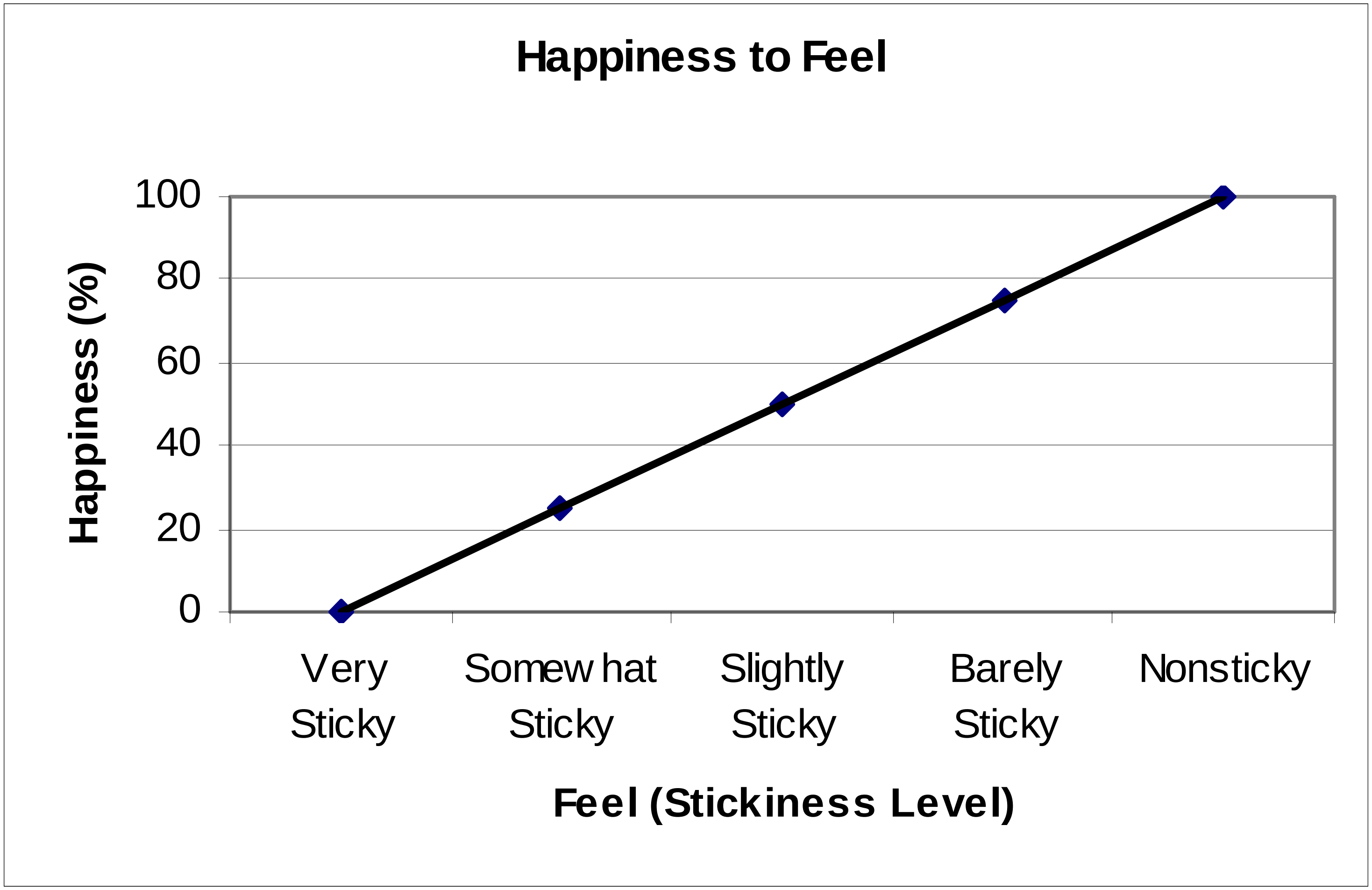
After correlating durability to several physical properties, initial vapor pressure of the mixture showed the strongest relationship.

This data was combined with the utility versus durability data to form a relationship between utility and mixture vapor pressure.

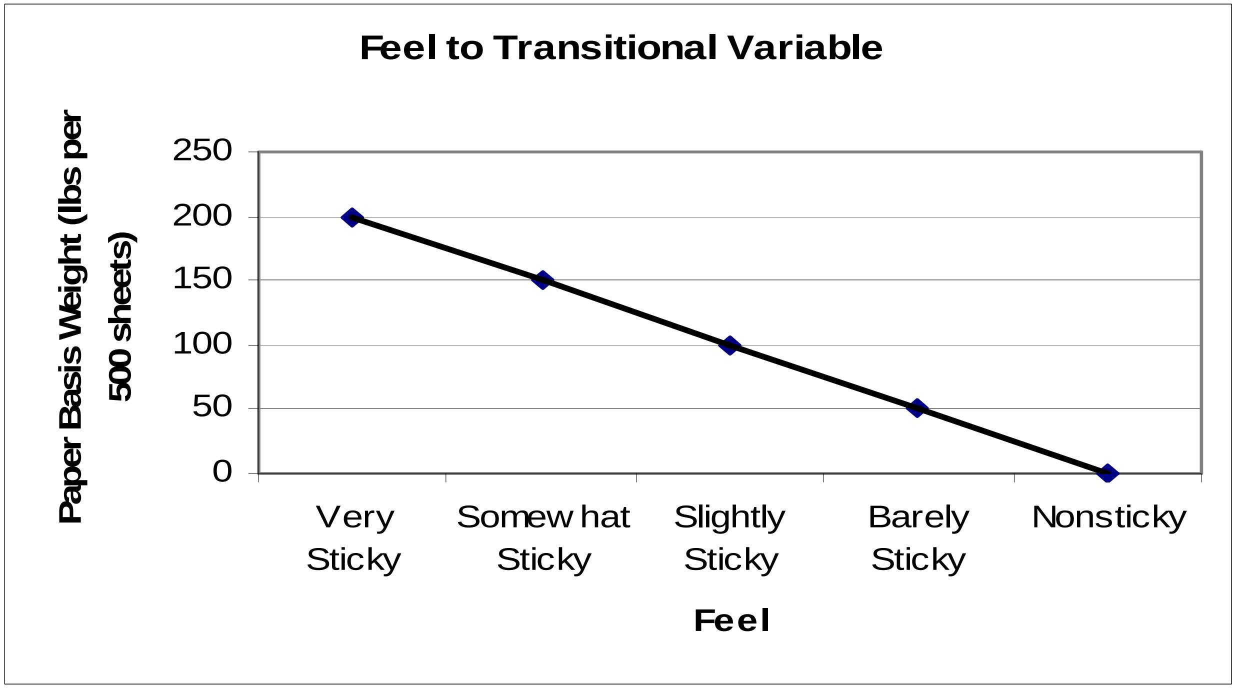
$$U = 100 - 9.664e^{3.72\times10^{-4}VP}$$

The Utility Function

Feel



The Utility Function
Feel



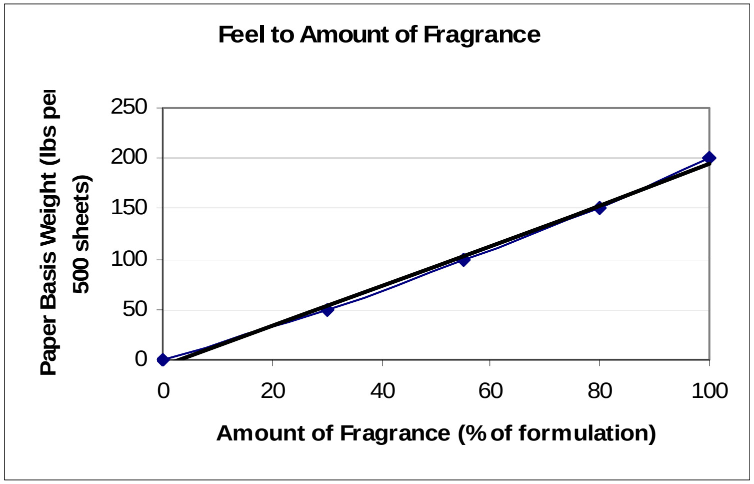
Paper basis weight: weight of 500 sheets of a certain paper thickness

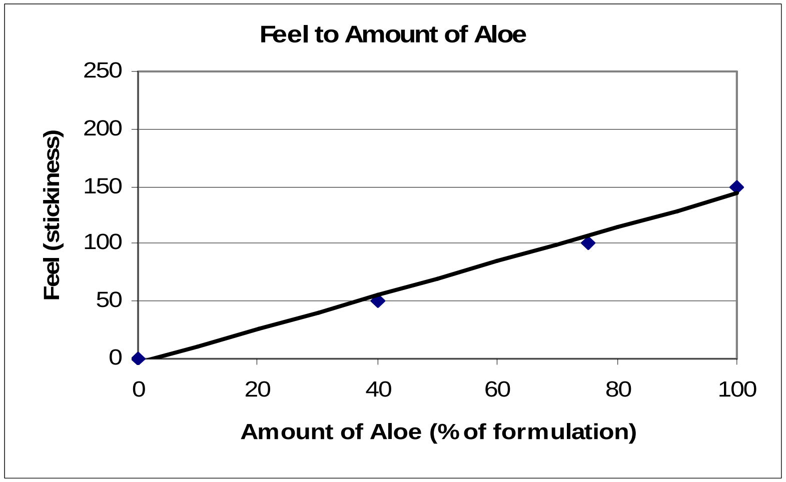
Aloe and Fragrance can leave a sticky residue when used in large amounts.

After applying a concentration of either component to the underside of the forearm, a 2” by 2” piece of paper is applied. The heaviest paper basis weight that will not fall off is used to describe the contribution of stickiness from each component to the final product.

The Utility Function

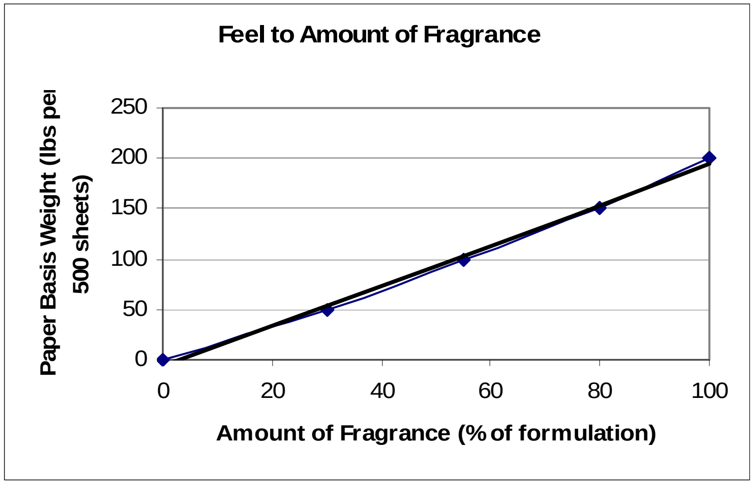
Feel

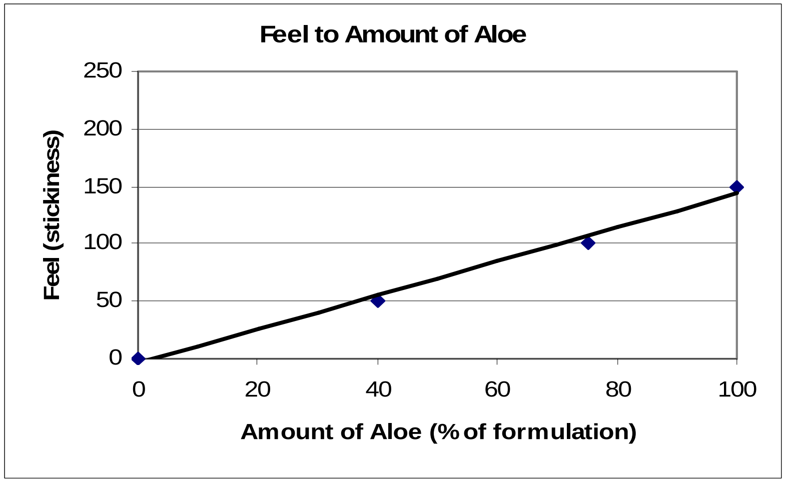


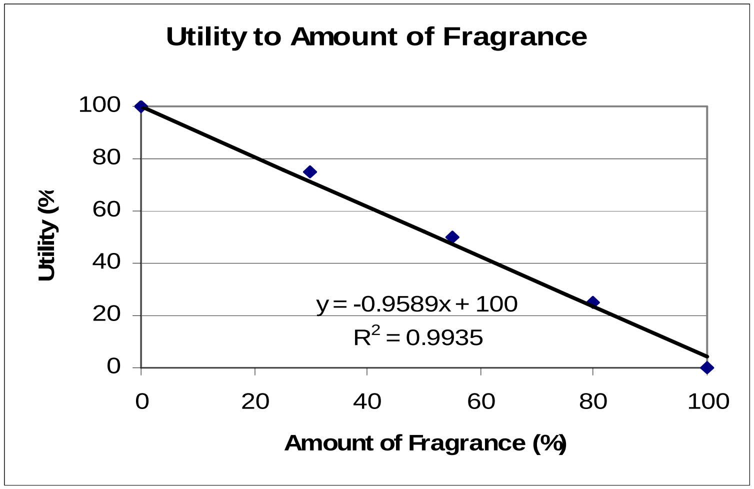


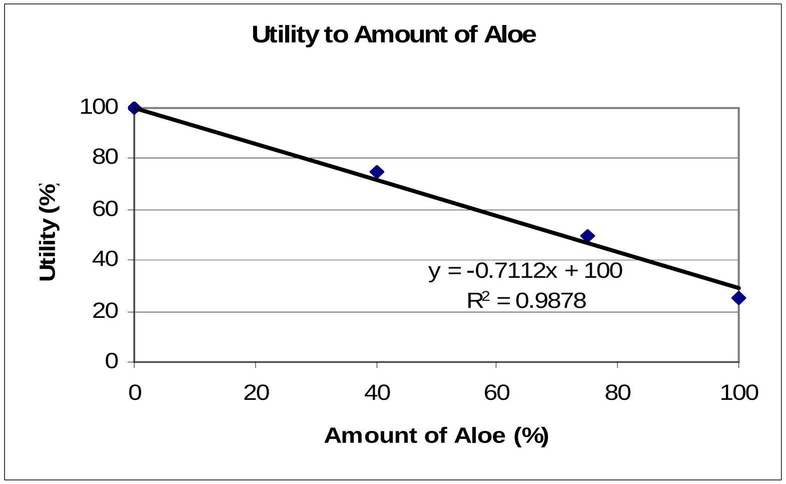
The Utility Function

Feel









The Utility Function

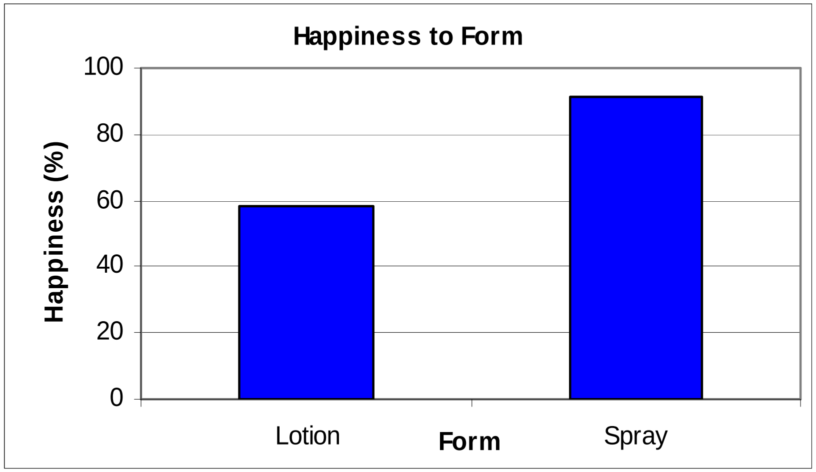
Feel

- Each ingredient contributes unequally to consumer utility
- Solution: weighted average
  - Each relationship has a y-intercept of 100, but differing rates of change:

$$U = 100 – (0.9589*x_{fragrance}) – (0.7112*x_{aloe})$$

The Utility Function

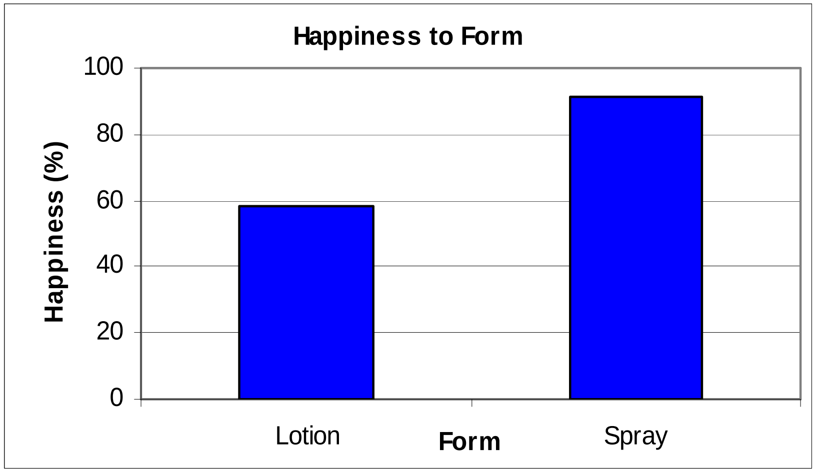
Form

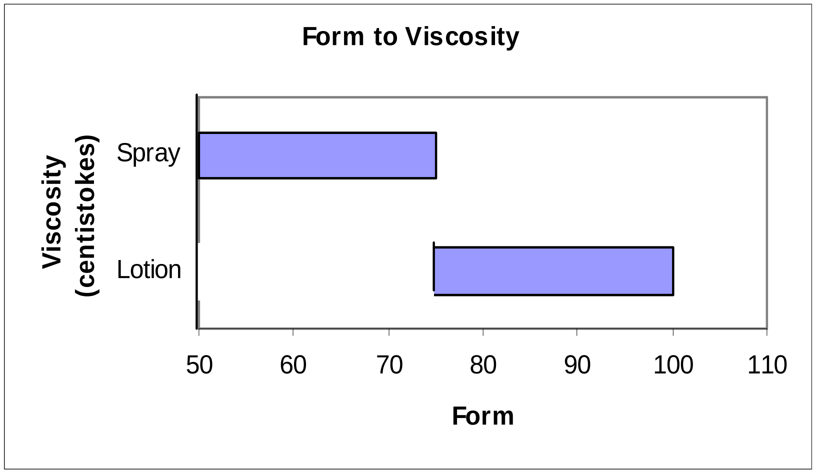


Market research data showed that 83% of consumers prefer spray repellent over the lotion form.

A repellent in spray form would give ‘100% happiness’ to 83% of consumers, but less happiness to the other 17%, approximated at 50%. Thus, a spray repellent would have an overall consumer utility of 92%.

The Utility Function
Form





Market research data showed that 83% of consumers prefer spray repellent over the lotion form.

A repellent in spray form would give '100% happiness' to 83% of consumers, but less happiness to the other 17%, approximated at 50%. Thus, a spray repellent would have an overall consumer utility of 92%.

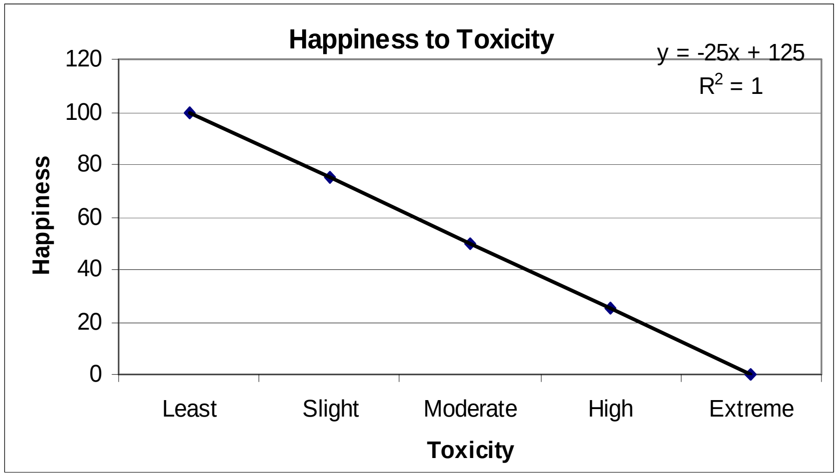
Liquids with a kinematic viscosity over 75 centistokes[1] will be too thick to be sprayed by a finger pump.

The relationship between form and utility can then be determined using an "If-Then" statement.

[1]www.jamestowndistributors.com/decoder_epifanestopcoats.jsp

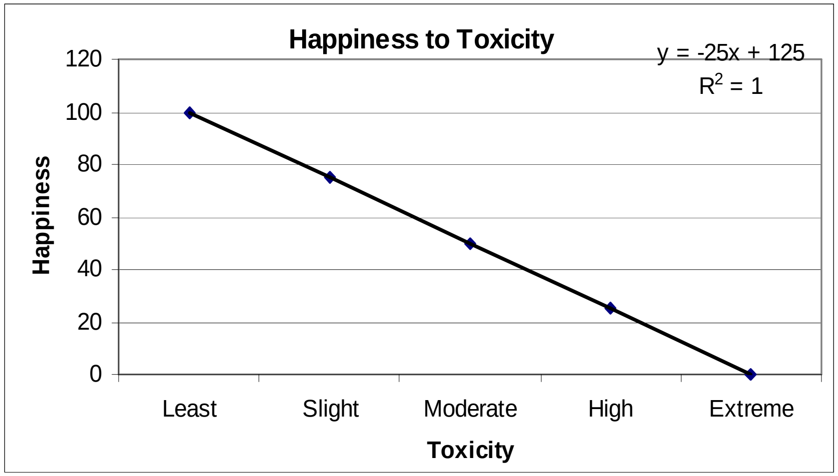
The Utility Function

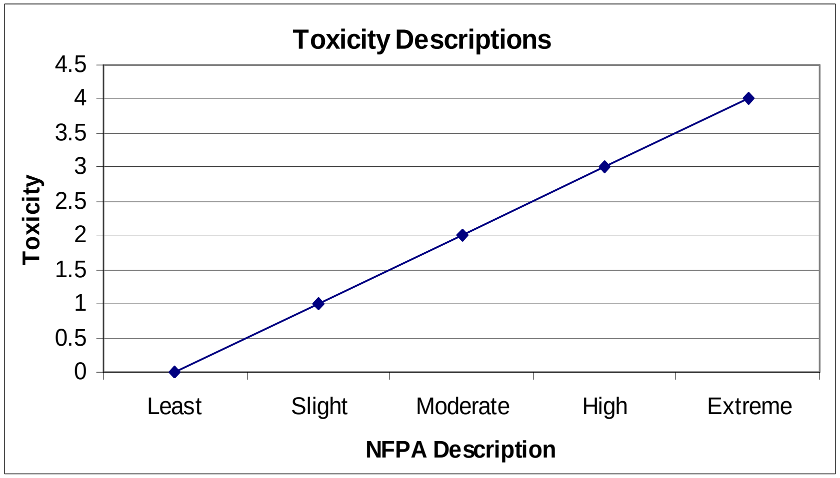
Toxicity



The Utility Function

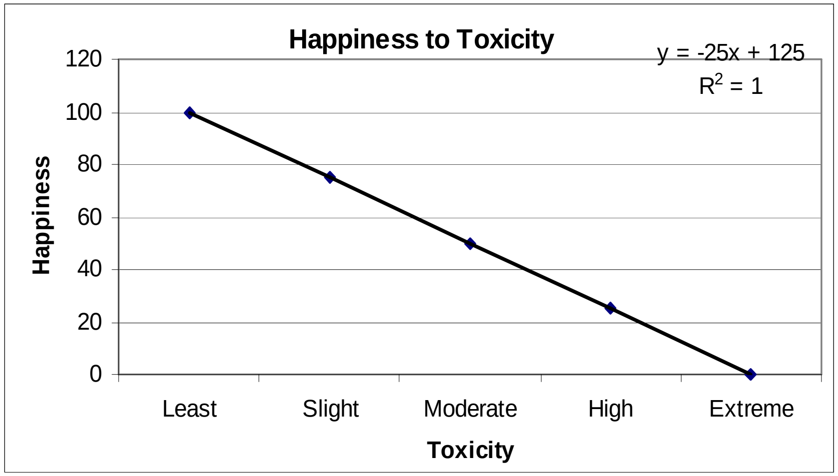
Toxicity

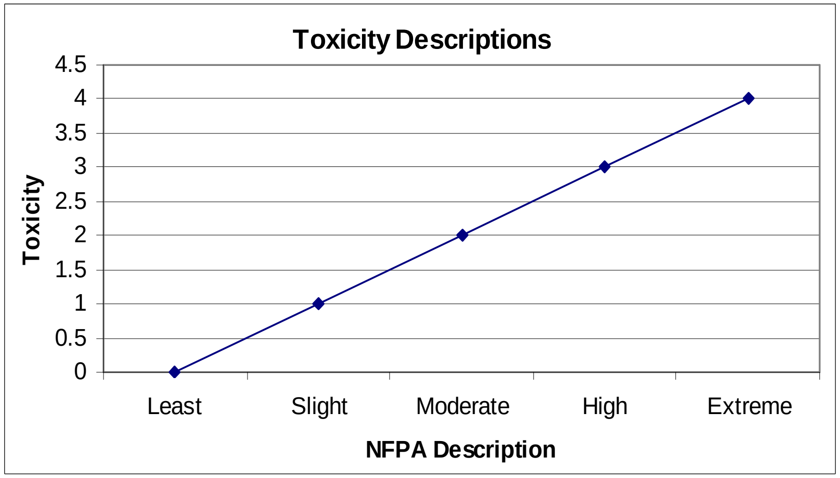


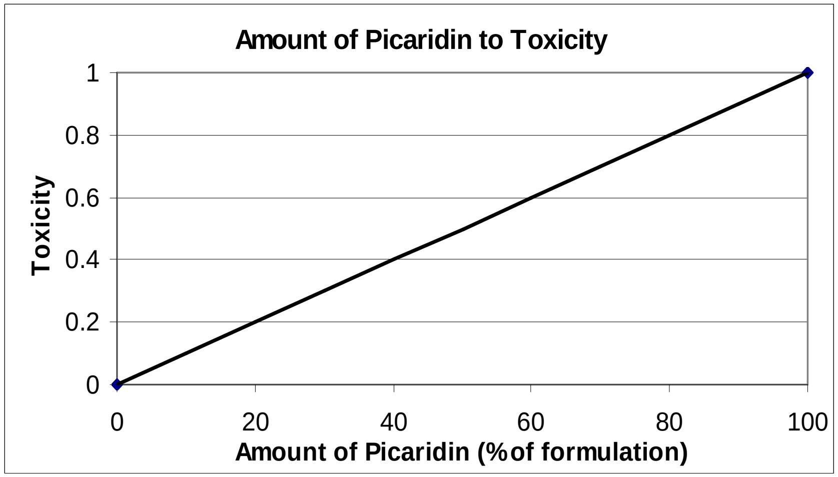


The Utility Function

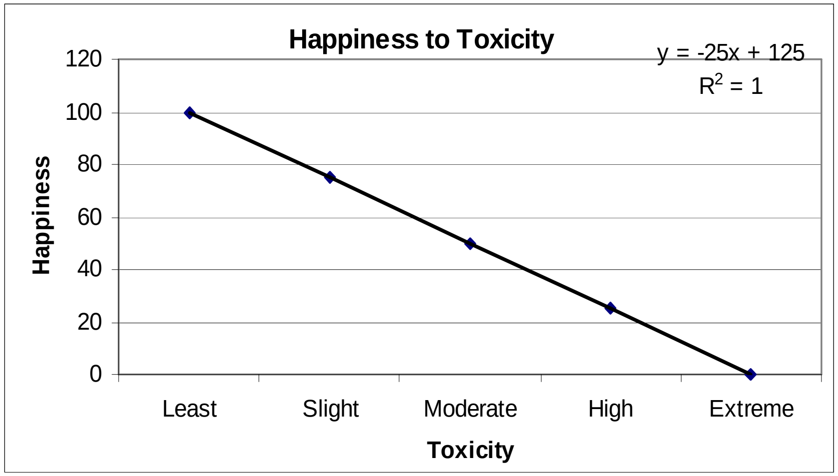
Toxicity

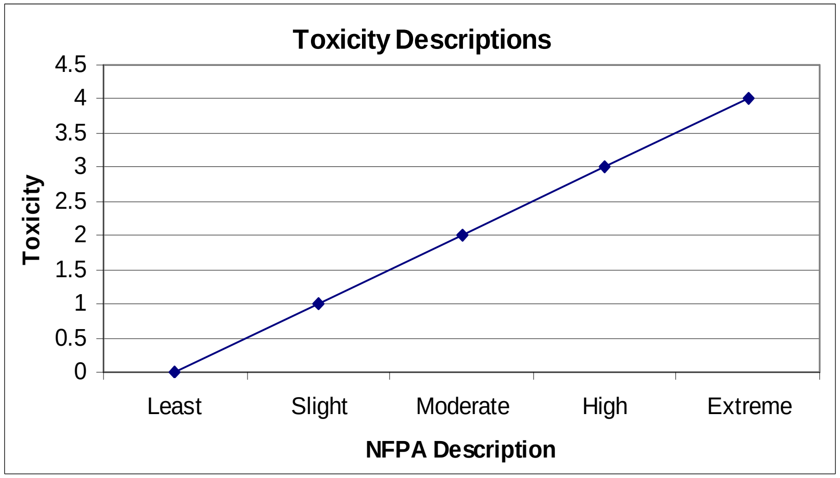


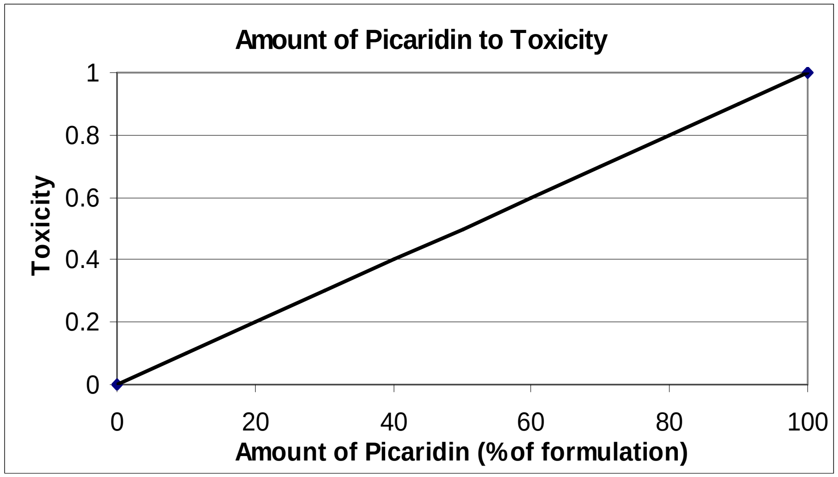


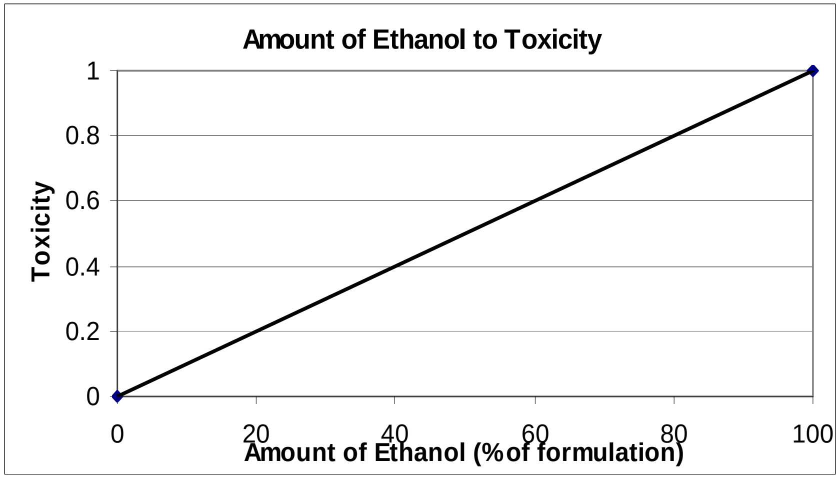


The Utility Function
Toxicity



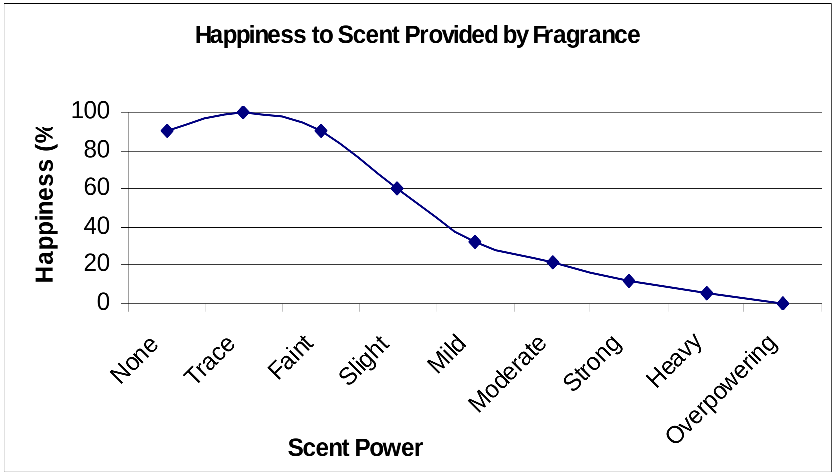






The Utility Function

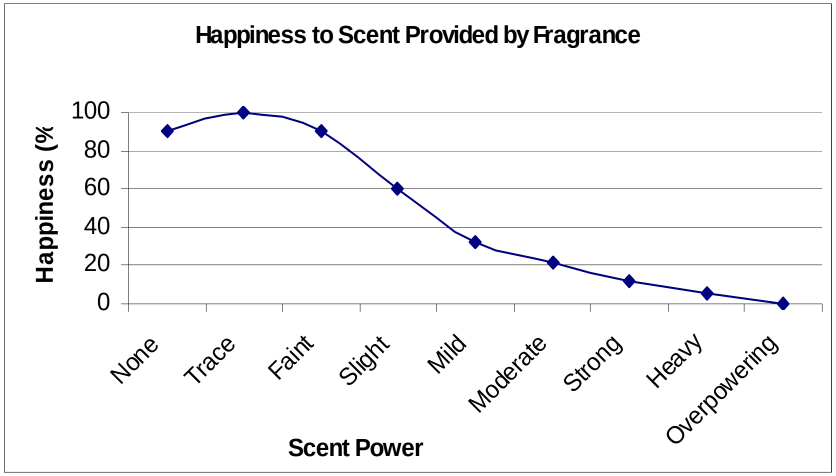
Scent

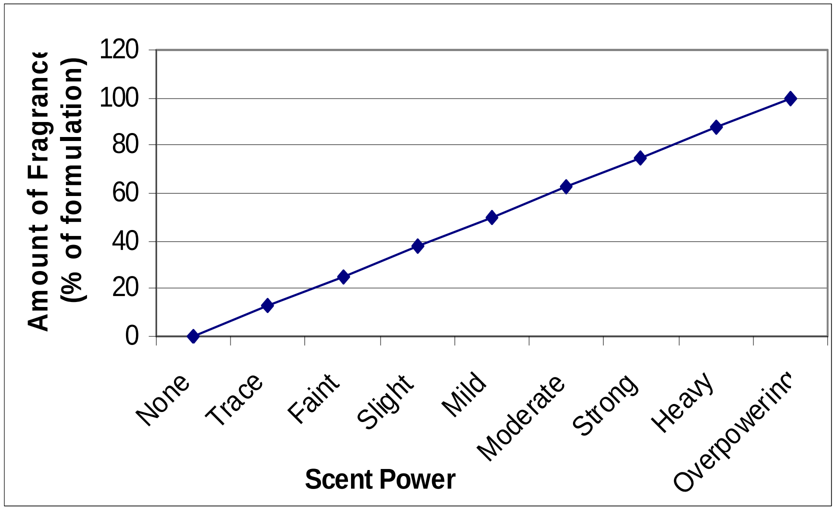


Qualitative scent description and utility

The Utility Function

Scent

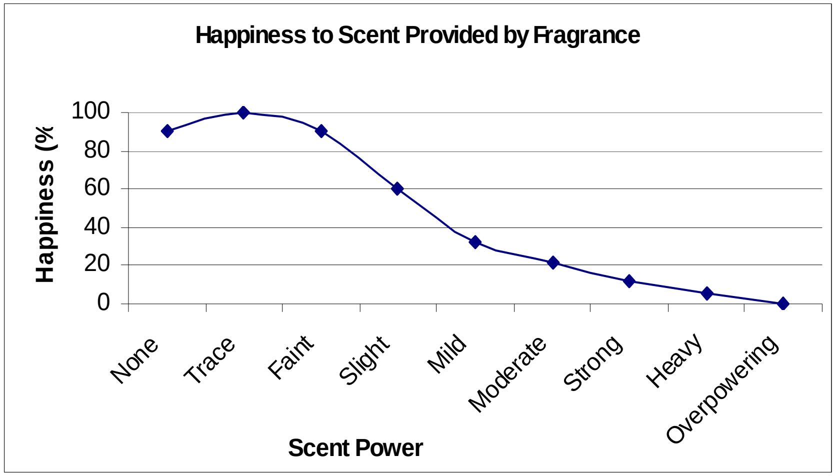




Qualitative scent description and utility + % fragrance and qualitative scent description

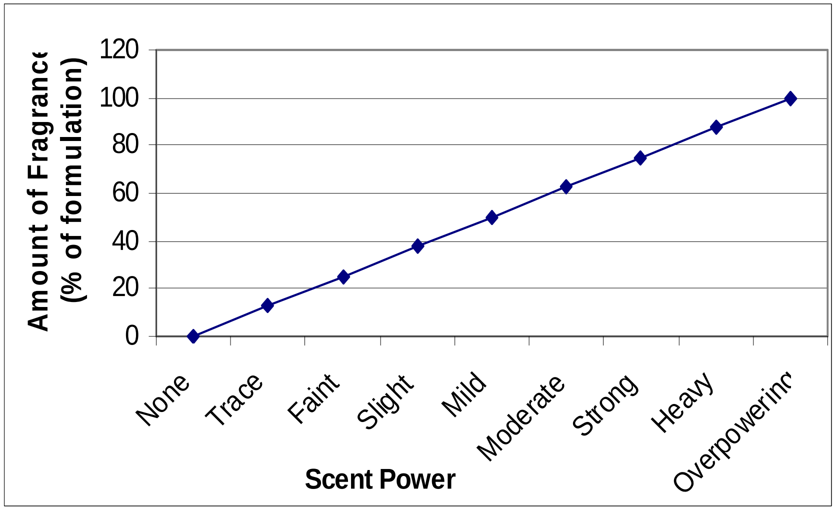
The Utility Function

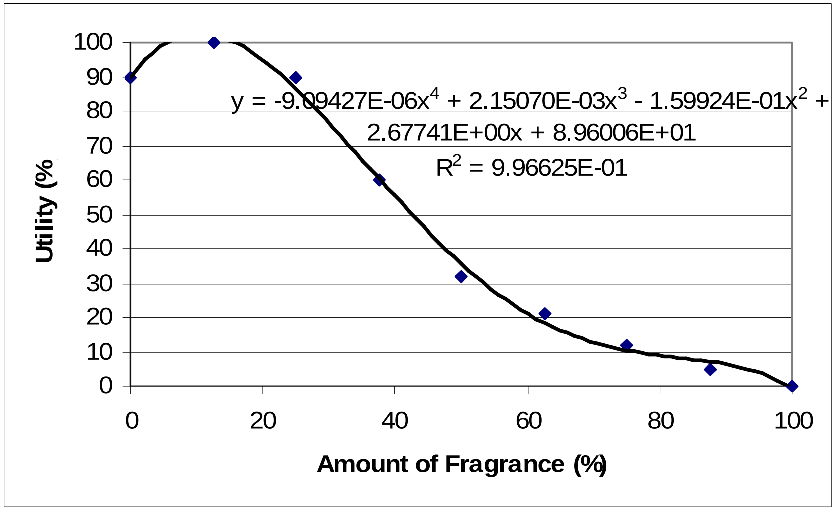
Scent



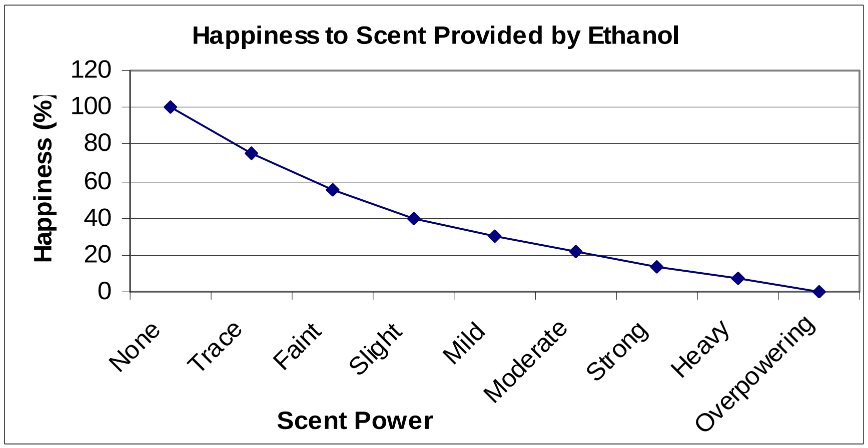
Qualitative scent description and utility + % fragrance and qualitative scent description → utility vs. % fragrance

$$U = -9.09E\text{-}06\ x^4 + 2.151E\text{-}03\ x^3 - 0.160\ x^2 + 2.677\ x + 89.6$$



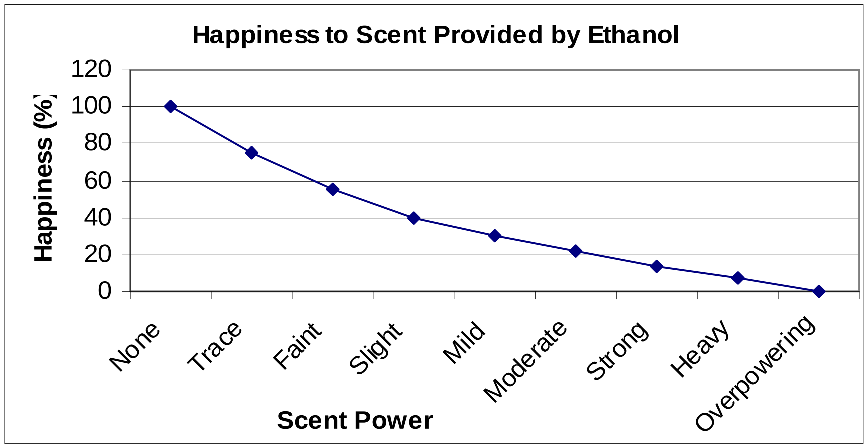


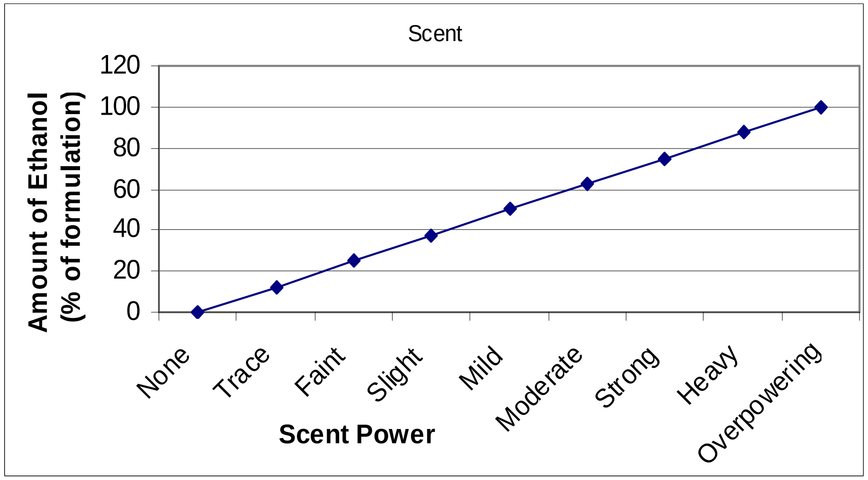
The Utility Function
Scent



Qualitative scent description and utility

The Utility Function
Scent

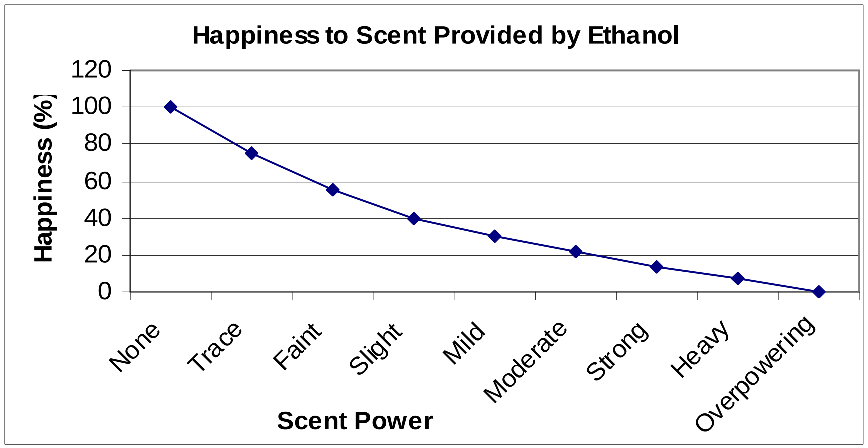




Qualitative scent description and utility + % ethanol and qualitative scent description

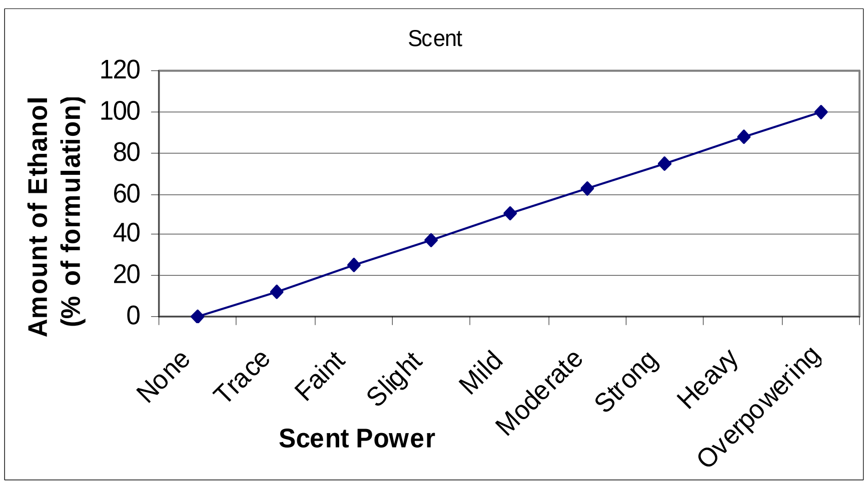
The Utility Function

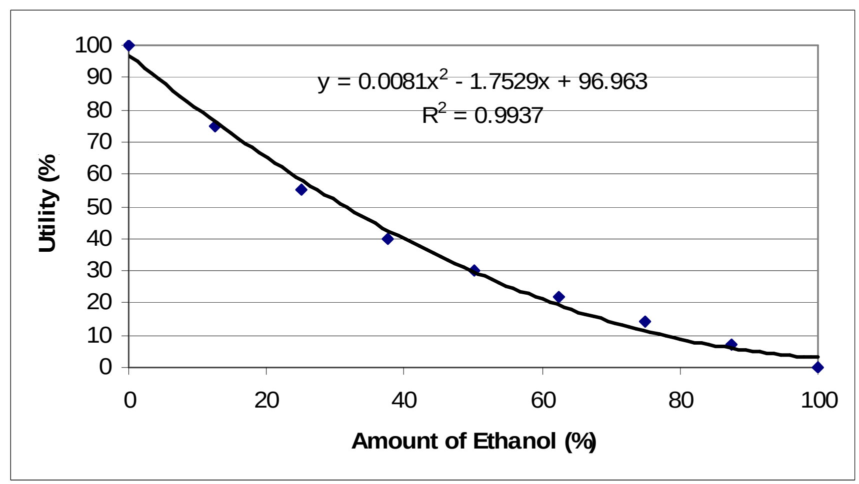
Scent



Qualitative scent description and utility + % ethanol and qualitative scent description → utility vs. % ethanol

$$U = 0.0081x^2 - 1.7529x + 96.963$$
$$R^2 = 0.9937$$





The Utility Function

Scent

- One ingredient has a positive effect, one has a negative effect on consumer utility

Solution:

Weighted average:

$$\frac{(U_{ethanol} * x_{ethanol} + U_{fragrance} * x_{fragrance})}{(x_{ethanol} + x_{fragrance})}$$

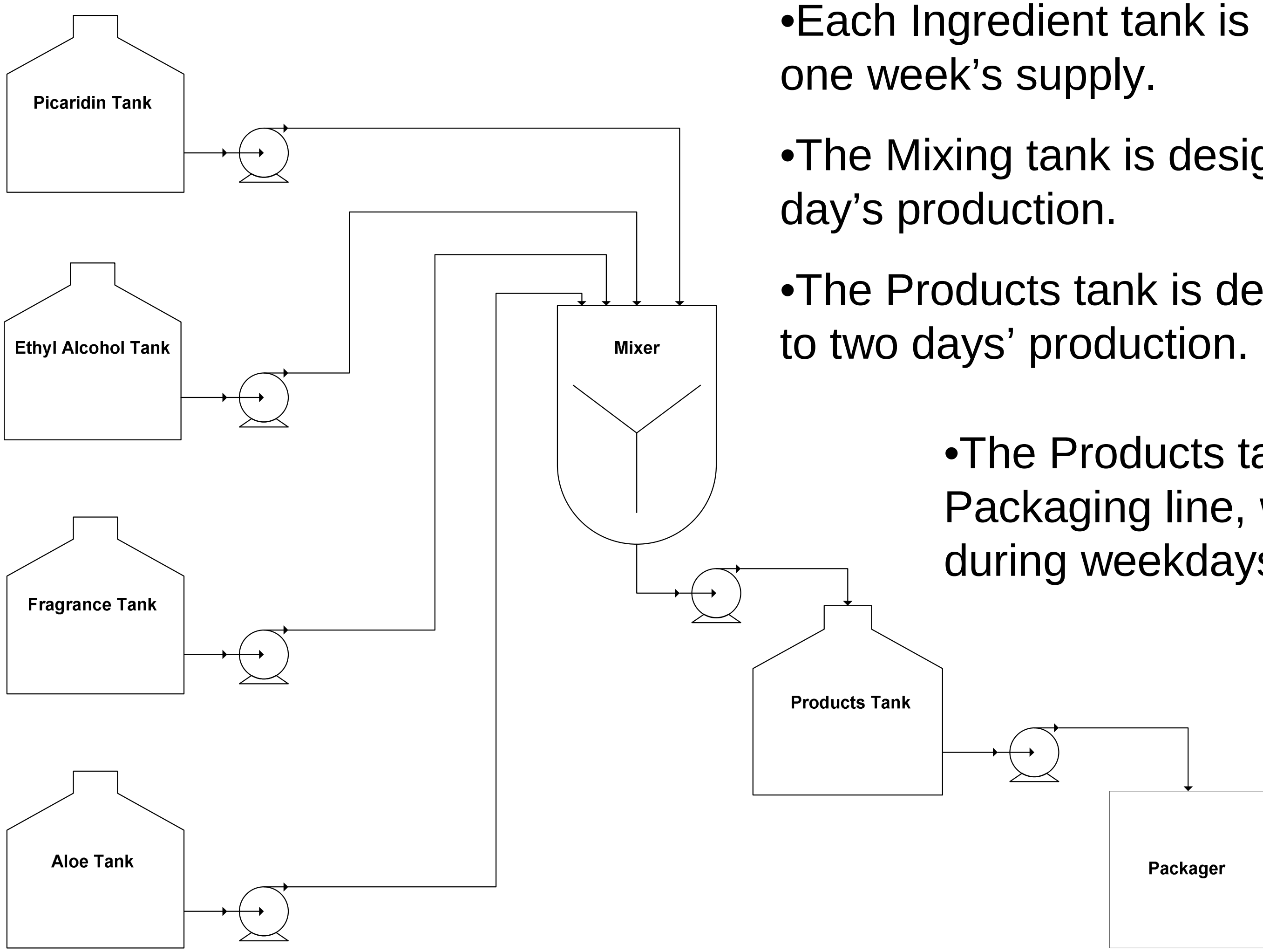
- Assumptions:

Picaridin, aloe are essentially odorless

Optimization
Cost Analysis

- Raw Material Costs
- Process Costs
  - All process equipment
  - Buildings
  - Utilities
  - Labor
- Shipping Costs
  - Optimized plant location: Little Rock, AR
  - Products shipped to 16 locations across the U.S.
- Advertising Costs
  - Annual budget set at $1 million

Optimization
The Production Process



- Each Ingredient tank is designed to hold one week's supply.
- The Mixing tank is designed to hold half a day's production.
- The Products tank is designed to hold up to two days' production.
- The Products tank feeds to the Packaging line, which is operated during weekdays only.

Optimization

Shipping

- Distribution centers were chosen to be able to cover all sections of the US.
- Percentage of production sent to each center was allotted to supply each region based on population and perceived need for the product.
- Assumptions: consumer utility is the same in each market (same target consumer); relative prices remain constant in each region; budget constraints have constant ratio to prices

CANADA
PACIFIC OCEAN
ATLANTIC OCEAN
GULF OF MEXICO
MEXICO
WASHINGTON
OREGON
IDAHO
MONTANA
WYOMING
NORTH DAKOTA
SOUTH DAKOTA
NEBRASKA
KANSAS
COLORADO
UTAH
NEVADA
CALIFORNIA
ARIZONA
NEW MEXICO
TEXAS
OKLAHOMA
MINNESOTA
WISCONSIN
MISSOURI
ARKANSAS
MISSISSIPPI
ALABAMA
GEORGIA
FLORIDA
ROCKY MOUNTAINS
GREAT PLAINS
LLANO ESTACADO
Lake Superior
Lake Ontario
Lake Erie
Gulf of California
BAJA CALIFORNIA
SONORA
CHIHUAHUA
COAHUILA
Chicago
New York
Boston
Los Angeles
San Diego
Phoenix
Houston
San Antonio
Jacksonville
El Paso
Winnipeg
Toronto
Montreal
POPULATED PLACES
1,000,000 and over
500,000 – 999,999
100,000 – 499,999
25,000 – 99,999
24,999 and less
National capital
State or provincial capital
Urban areas
Chicago
Seattle
Omaha
Flagstaff
Washington
Albany
TRANSPORTATION
Interstate; limited access highway
Other principal highway
Ferry
Railroad
PHYSICAL FEATURES
Streams: perennial; intermittent
Lakes: perennial; intermittent
Bathymetry (meters)
Highest elevation in state (feet)
Other elevations (feet)
Forest cover
STANDARD TIME ZONES
SCALE 1:5,000,000
Compiled by U.S. Geological Survey
2001
Principal Islands of HAWAII
Puerto Rico and the Virgin Islands

Optimization

Shipping

Distribution Center	Percent of Production Received	Shipping Distance
Eugene, OR	5	1752
Salt Lake City, UT	5	1144
Denver, CO	5	1635
Lubbock, TX	6	767
Kansas City, MO	7	551
Indianapolis, IN	7	326
Jacksonville, FL	7	484
Albany, NY	7	683
Sacramento, CA	7	1133
Phoenix, AZ	6	1142
Billings, MT	6	1132
Baton Rouge, LA	7	304
St Paul, MN	6	706
Memphis, TN	7	129
Charlotte, NC	7	648
Pittsburgh, PA	5	779

Optimization
Shipping

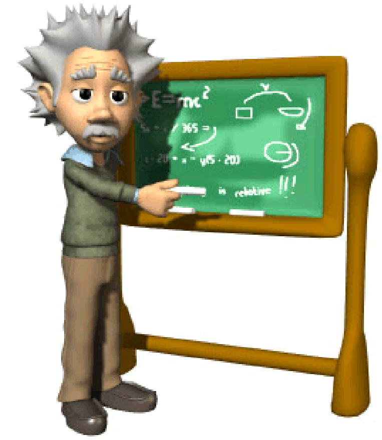
Location	Shipping Costs
Oklahoma City, OK	$25,680
Lafayette, LA	$26,611
Shreveport, LA	$26,067
Jackson, MS	$25,919
Birmingham, AL	$26,006
Little Rock, AR	$25,243

Source: uams.edu

Costs shown are per ton of production.

This optimization showed that Little Rock, AR would be the best location for constructing our plant.

Optimization
Economic Analysis



Source: http://www.bytefusion.com/products/ens/secexmail/smart_guy_teaching_hr.gif

- Budget Constraint:

$$P_1D_1 + P_2D_2 \leq Y$$

P is price; D is demand; Y is budget constraint; 1 is our product; 2 is the competition

- Price and Demand:

$$\beta P_1D_1 = \alpha P_2D_2D_1^{\alpha}/D_2^{\beta}$$

β is relative utility; α is relative consumer awareness

Optimization
Economic Analysis

- Algebraic manipulation and substituting for D_2 gives:

$$D_1^{1-\alpha} = \left(\frac{\alpha P_2}{\beta P_1}\right)\left(\frac{Y - P_1 D_1}{P_2}\right)^{1-\beta}$$

(LHS) (RHS)

- If the other parameters are given, the D_1 that makes this equation true is our annual production.

Optimization
Procedure

- Demand Equation: $$D_1^{1-\alpha} = \left(\frac{\alpha P_2}{\beta P_1}\right)\left(\frac{Y - P_1 D_1}{P_2}\right)^{1-\beta}$$
- α: relative consumer awareness, set at 0.9
- β: relative utility = U_2/U_1
  - U_1: combined utility of our formula
  - U_2: combined utility of competitor's formula
- Y: market budget constraint
- P_2: price of competitor

Optimization
Procedure

$$D_1^{1-\alpha} = \left(\frac{\alpha P_2}{\beta P_1}\right)\left(\frac{Y - P_1 D_1}{P_2}\right)^{1-\beta}$$

- Set P_1 and D_1
- Guess a composition of repellent formula
  - U_1 is calculated from this
  - β is calculated from U_1
- Set up two cells in Excel: LHS and RHS of demand equation
- Enter all economic formulas into Excel, set to automatically calculate based on D_1
  - Annual Revenue
  - Annual Return on Investment
- Use Excel Solver to set LHS and RHS cells equal to each other by changing concentration
- Repeat for different D_1's
- Repeat for different P_1's

Maximized Utility Product

- When utility is maximized:
  - 93.6% Utility
- Resulting composition:
  - Picaridin: 98%
  - Aloe: 0%
  - Ethanol: 2%
  - Fragrance: 0%
- Cost to break even:
  - Over $60 a pound

Source: http://www.parktudor.pvt.k12.in.us/innell/smiling%20sun.gif

Maximized Utility Product

- We want to make this product profitable.

- From market analysis,
  - Market budget constraint: $25 million per year
  - Competitor: Deep Woods OFF! for Sportsmen
    - 100% DEET
    - $96.00 per pound

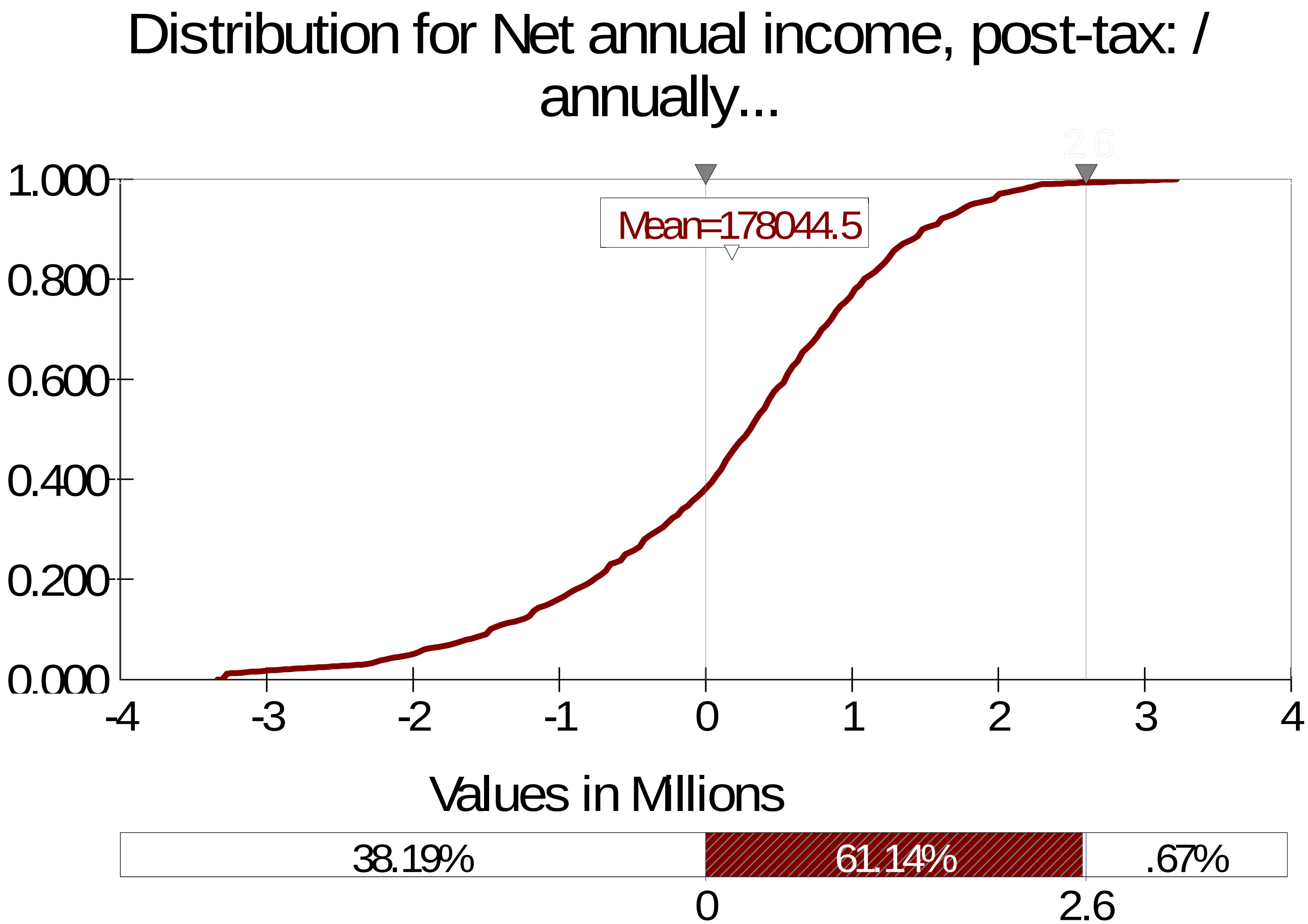
Maximized Utility Product

- This product can be profitable!
  - Demand: 125,000 pounds per year
  - Price: $80 per pound ($5 per 1 oz. bottle)
  - Net Income: $310,000 per year

- However, raw material costs are the largest cost, so any deviations in these could have a large effect.

Maximized Utility Product

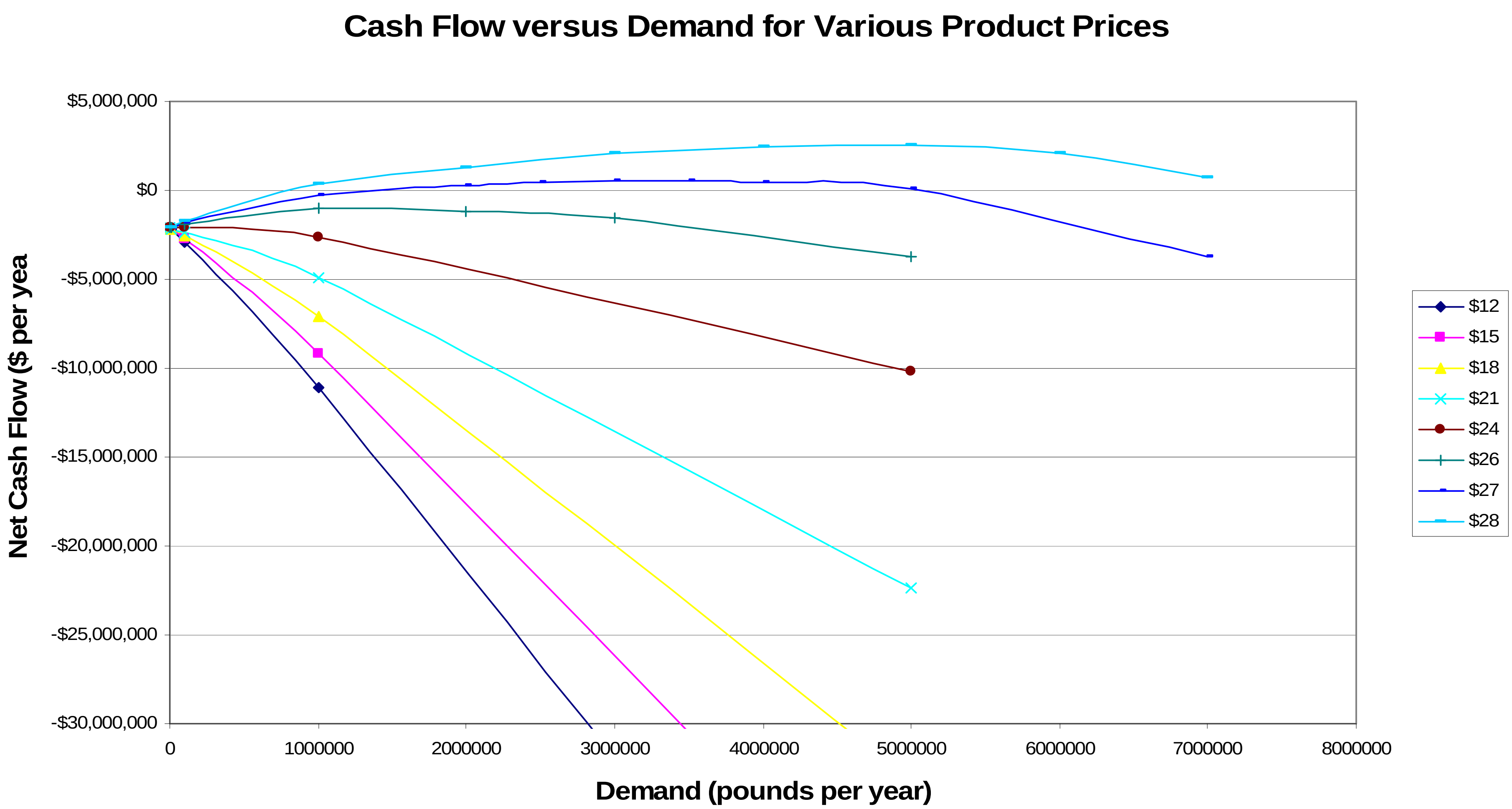
Risk Analysis



Maximizing Profit

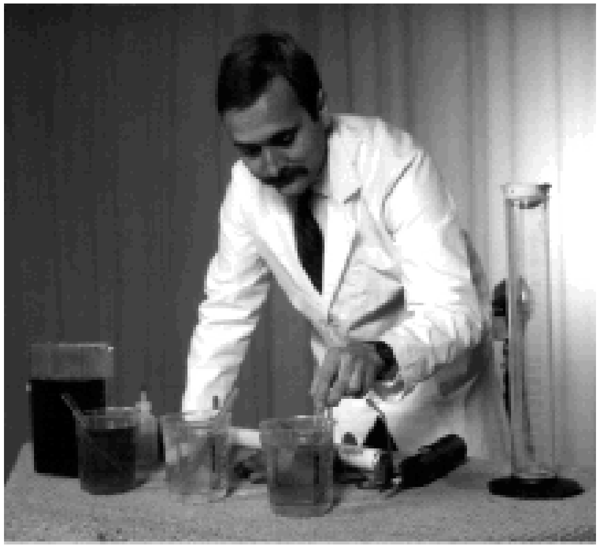
- The previous approach was deemed too risky, so it was decided to develop a product with a larger consumer pool.
- New aim: common repellents
  - Less effective
  - Less expensive
- New market budget constraint: $250 million per year
- New competitor: Cutter Advanced
  - 7% Picaridin
  - $16.00 per pound

Maximizing Profit



Maximized Profit Product

- Resulting composition
  - Picaridin: 43%
  - Aloe: 1%
  - Ethanol: 55%
  - Fragrance: 1%



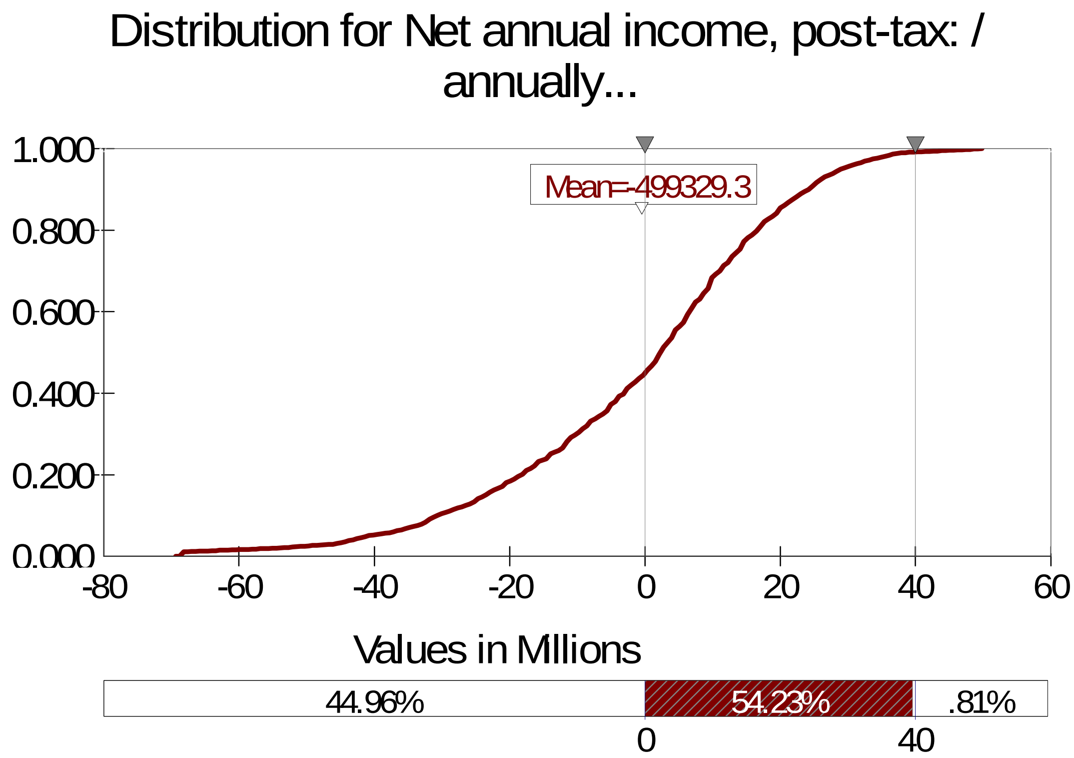
Source: http://www.mobileedproductions.com/images/chem1bandw.gif

- Demand: 5 million pounds per year
- Price: $28 per pound ($10.50 per 6 oz. bottle)
- Net Income: $2.55 million per year

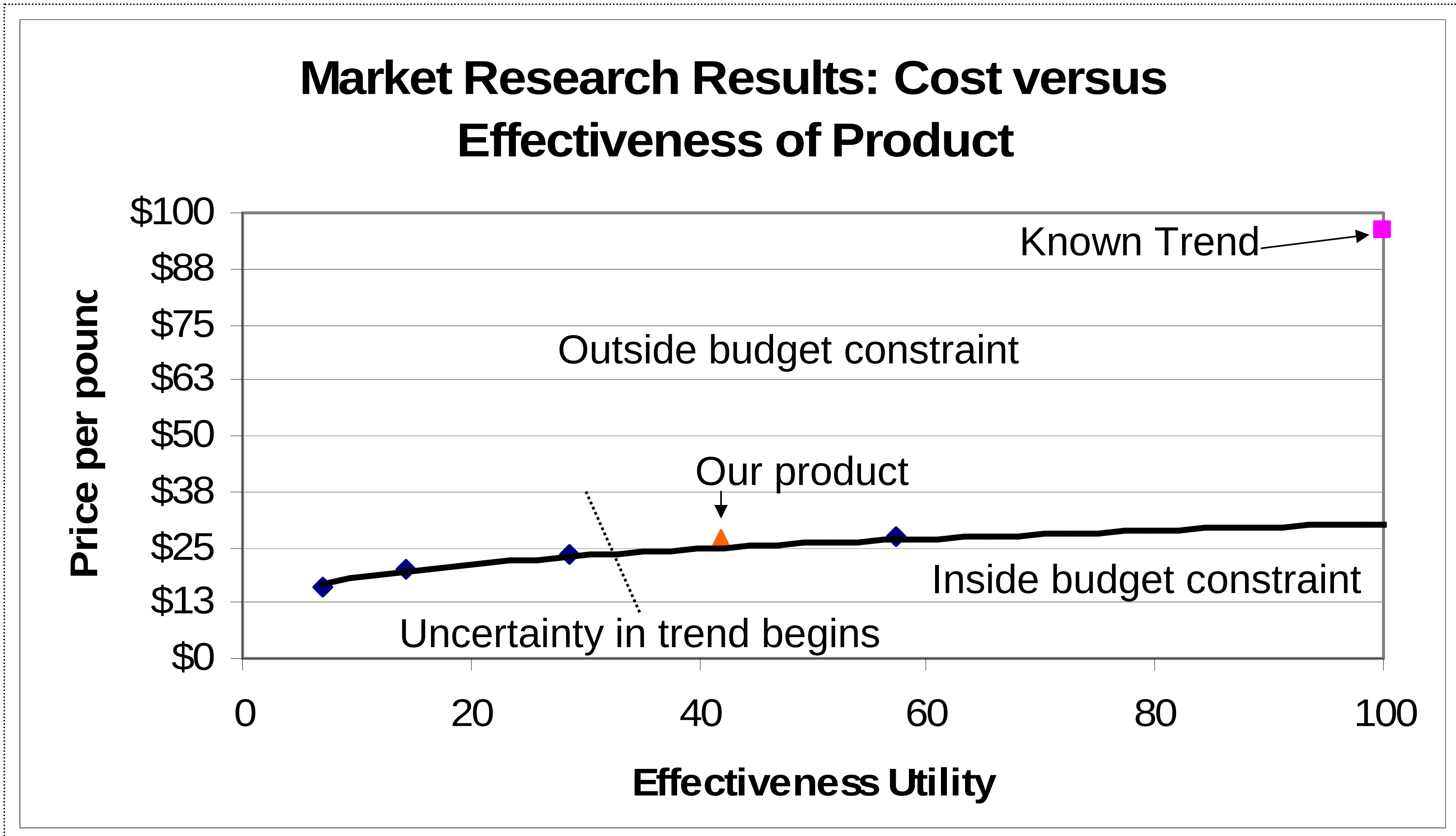
Maximized Profit Product

Risk Analysis

- A standard deviation of 20% was assumed in the raw materials costs
- 55% chance of our product being profitable
- Expected profit is -$500,000



Consumer Budget Constraint



Conclusions

Source: http://www.oc88.com

- The Safer Choice
  - Market the specialty repellent
    - Less risk involved
    - Less profit possible (millions)
- The More Lucrative Choice
  - Market the common repellent at a higher price
    - Riskier
    - Higher possible profit (10s of millions)
    - Because of uncertainty of budget constraint, further market research should be performed

Environmental Impact

- Production only involves mixing
  - No gas releases
  - No harmful byproducts
- All ingredients non-toxic
  - Leaks present no serious environmental concerns
- Largest impact is related to shipping (truck emissions)

Source: http://residentialvessels.com/environment.htm

Recommendations for Future Work

- Marketing Survey
  - Revise to include “form”
  - Increase sample size
  - Refine budget constraint

- Production
  - Investigate synthesis of Picaridin
- Miscellaneous
  - Find more accurate costs and physical property data

Any Questions?