

Slow Release Fragrance and Disinfectant for Carpets

ChE 4273 Capstone
Dr. Bagajewicz

Justin Woody
Carrie Street

Overview

- Background
- Design
- Utilities
- Production Process
- Economics

The Case for a Clean Carpet

- Dust Mites
- Mold
- Mildew
- Bacteria



Dust Mites



- Microscopic arachnids
- Dust mite's dead remains and fecal matter are invisible cause respiratory problems
- Remains are suspended in the air for extended periods of time

Dust Mites: Ideal Environment

- Feed on dead human skin cells

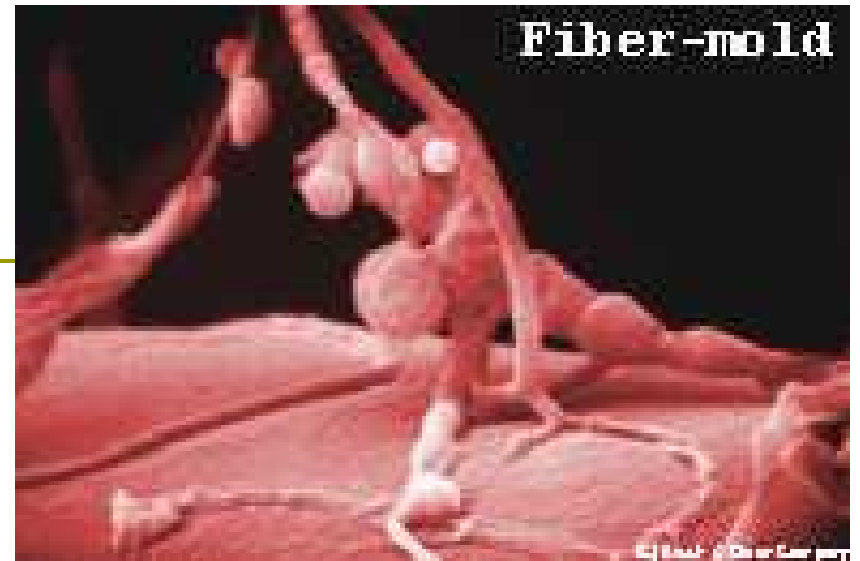
- $> 55\%$ humidity

- 72° - 79° F

- $< 50\%$ humidity, most die within 7-10 days

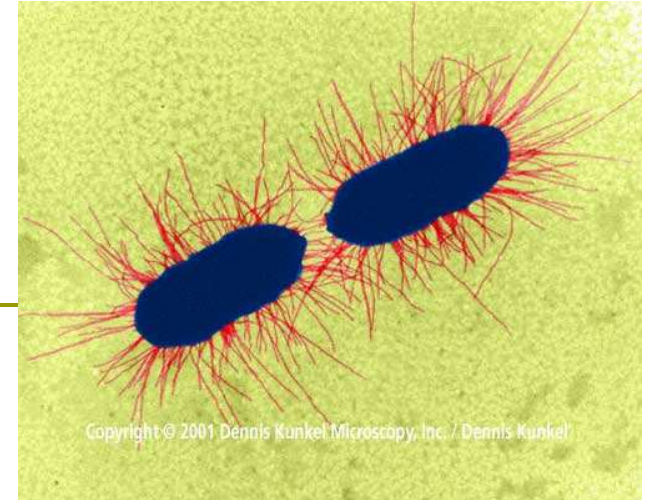


Mold & Mildew



- Moist, warm, poorly ventilated places
- Quickly mature
- Produce floating spores
- Cause discomfort and allergies

Bacteria



- Gram negative
- Anaerobic
- Require wet environment
- Live in latex backing of carpet
- Produce butyric acid – foul smell

Wet Cleaning Problems

- Cause mildew growth
- Up to 20% water absorption
- Analogous to shampooing hair without rinsing
- Soapy, sticky residue



Current Products

□ Arm&Hammer



www.churchdwright.com

□ Borid



www.pestproducts.com

□ Capture Clean



www.captureclean.com

Challenge

Freshen and Disinfect – With Powders

- Slow release fragrance
- Small particles (biodegradable)
- Disinfectant

Problem

Potential Solution

Dust Mites

boric acid, tannic acid

Mold

boric acid, sodium propionate

Bacteria

neutralize butyric acid odor with **baking soda**

Mildew

boric acid, baking soda

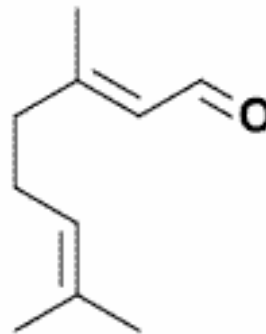
Natural Fragrances

Linalool



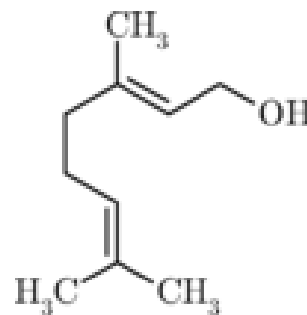
Lily

Citral



Lemon

Geraniol



Rose

Design

- Baking Soda
- Boric acid
- Linalool in PLGA for *extended duration*

Sodium bicarbonate

- Absorbs moisture
- Non-toxic

Boric Acid

- Kill dust mites
 - crystal coats food source
- Neutralize allergens
- Inhibit mold, mildew, bacteria, and fungi growth
- Kill cockroaches, beetles, and ants by chemical burns

BORON COMPOUND

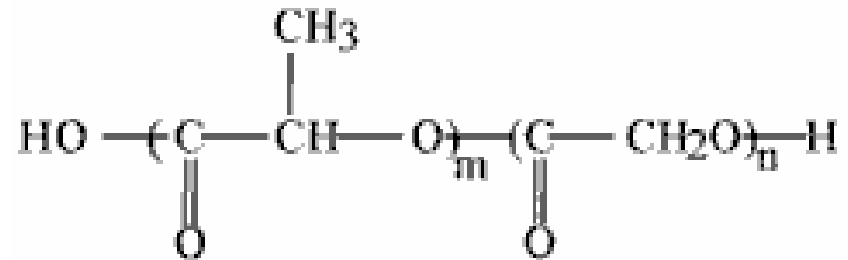
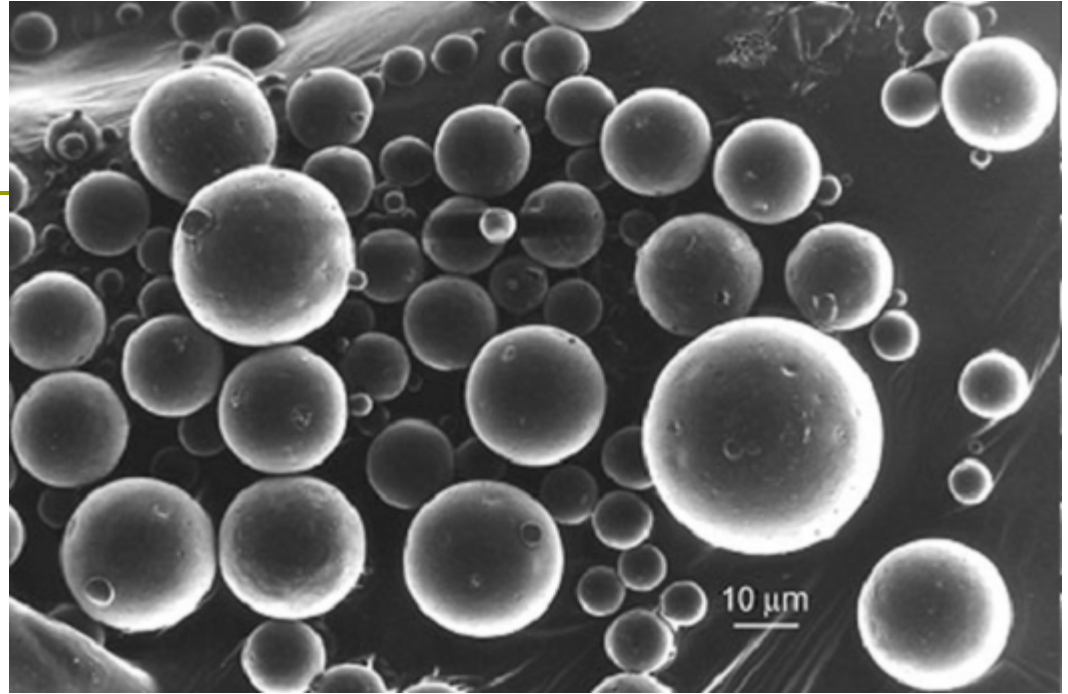
As Found In DUSTMITE AND FLEA CONTROL™

Dust Mite's Food Source
Becomes Coated And
Mites Eventually Die



PLGA

- Poly(lactic-co-glycolic acid)
- Biodegradable
- Degrades by hydrolysis of ester linkages



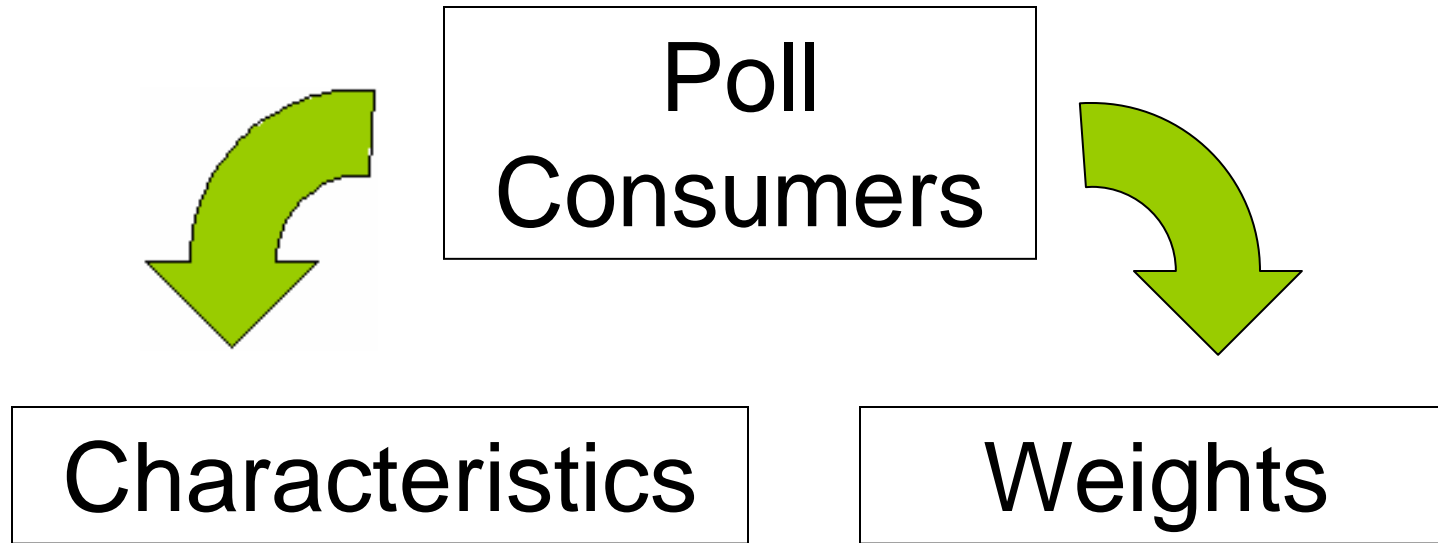
Utility Function Method

$$U = \sum U_i w_i$$

U = utility w = importance weight

i = characteristic

Utility Function Method



$$\sum \text{weights} = 1$$



Characteristic	Weight
Disinfectant Effectiveness	0.21
Scent Intensity	0.22
Fragrance Duration	0.19
Toxicity	0.09
Odor Elimination	0.15
Scent Type	0.14

Utility Function Method



Consumer
Tests

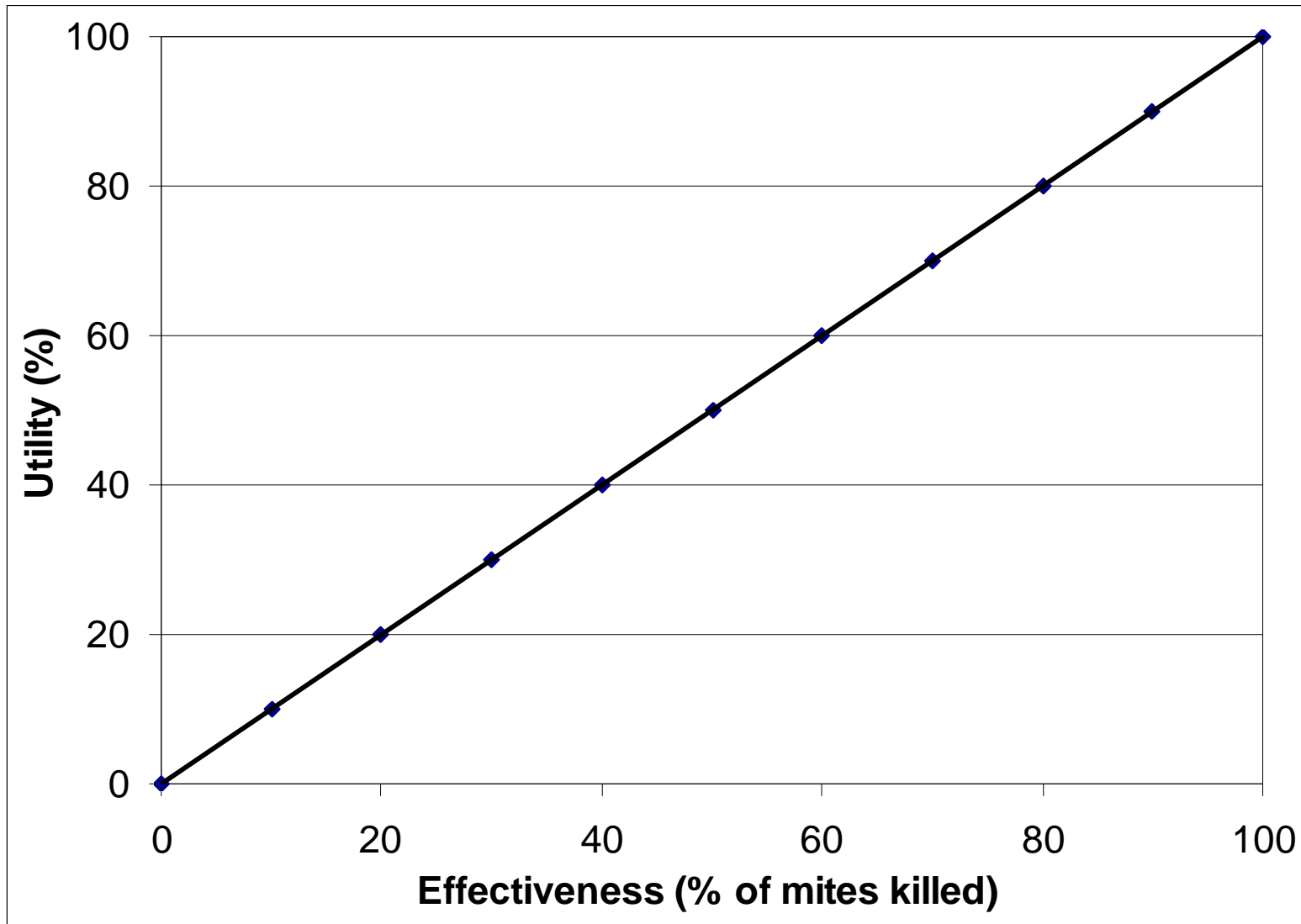
measure preference

Relate characteristics to
physical property

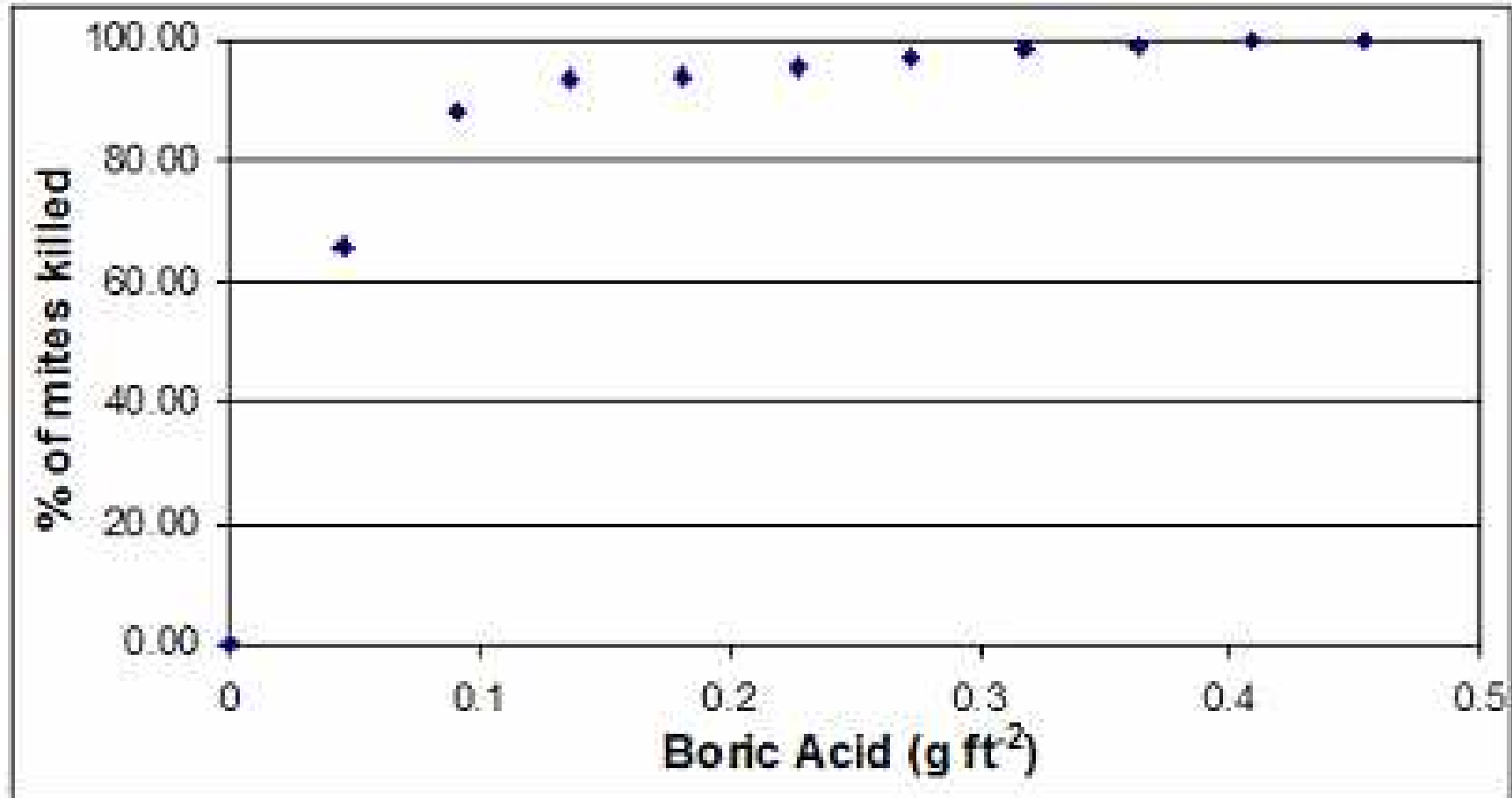
Disinfectant Effectiveness relates

- % of mites killed
- Amount of boric acid per unit area

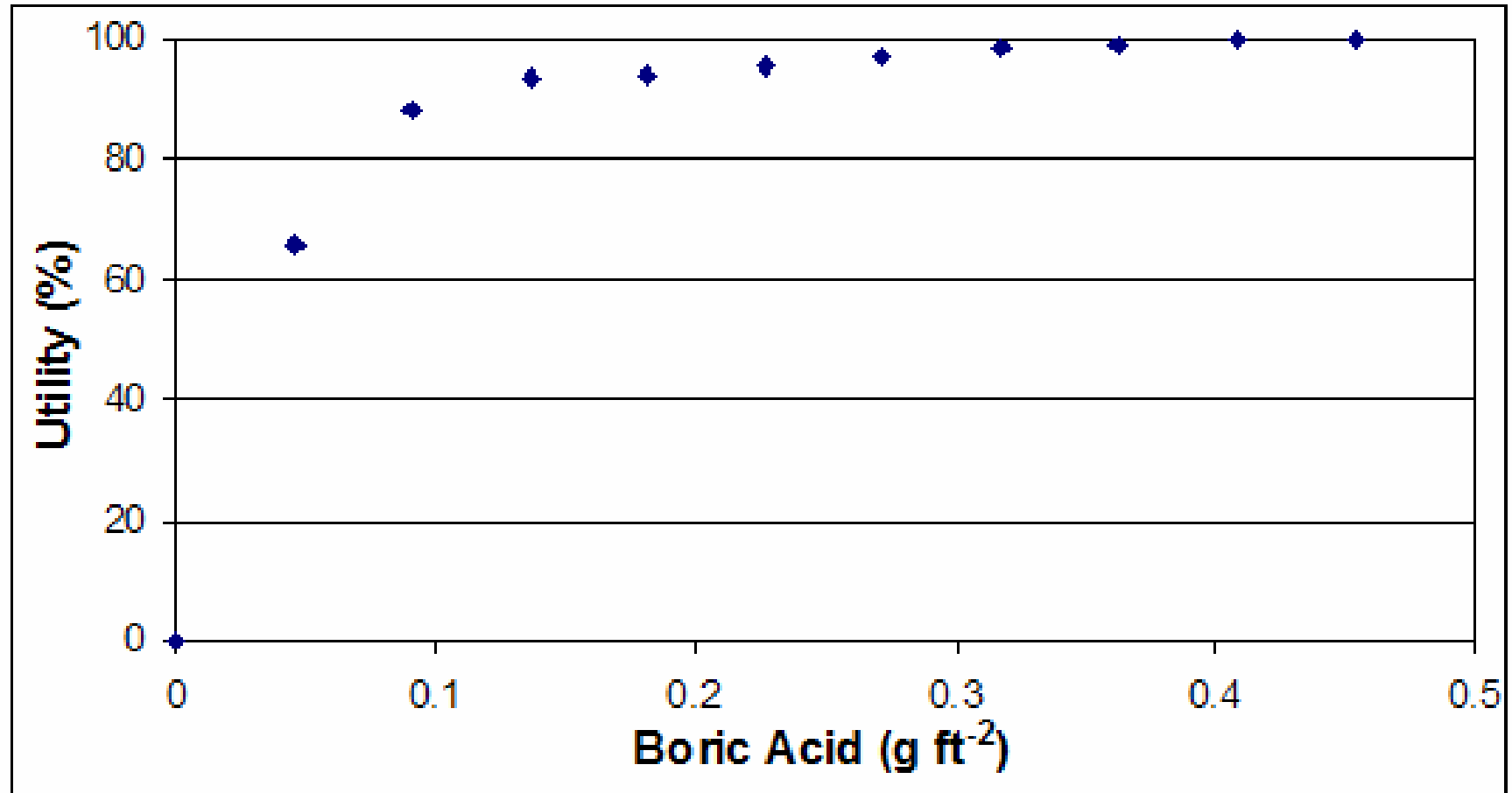
Disinfectant Effectiveness



Disinfectant Effectiveness

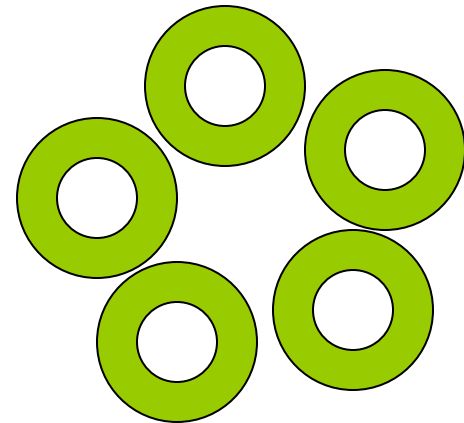
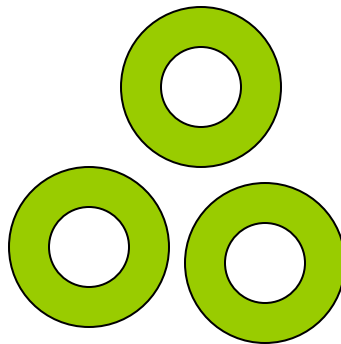
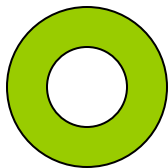


Disinfectant Effectiveness

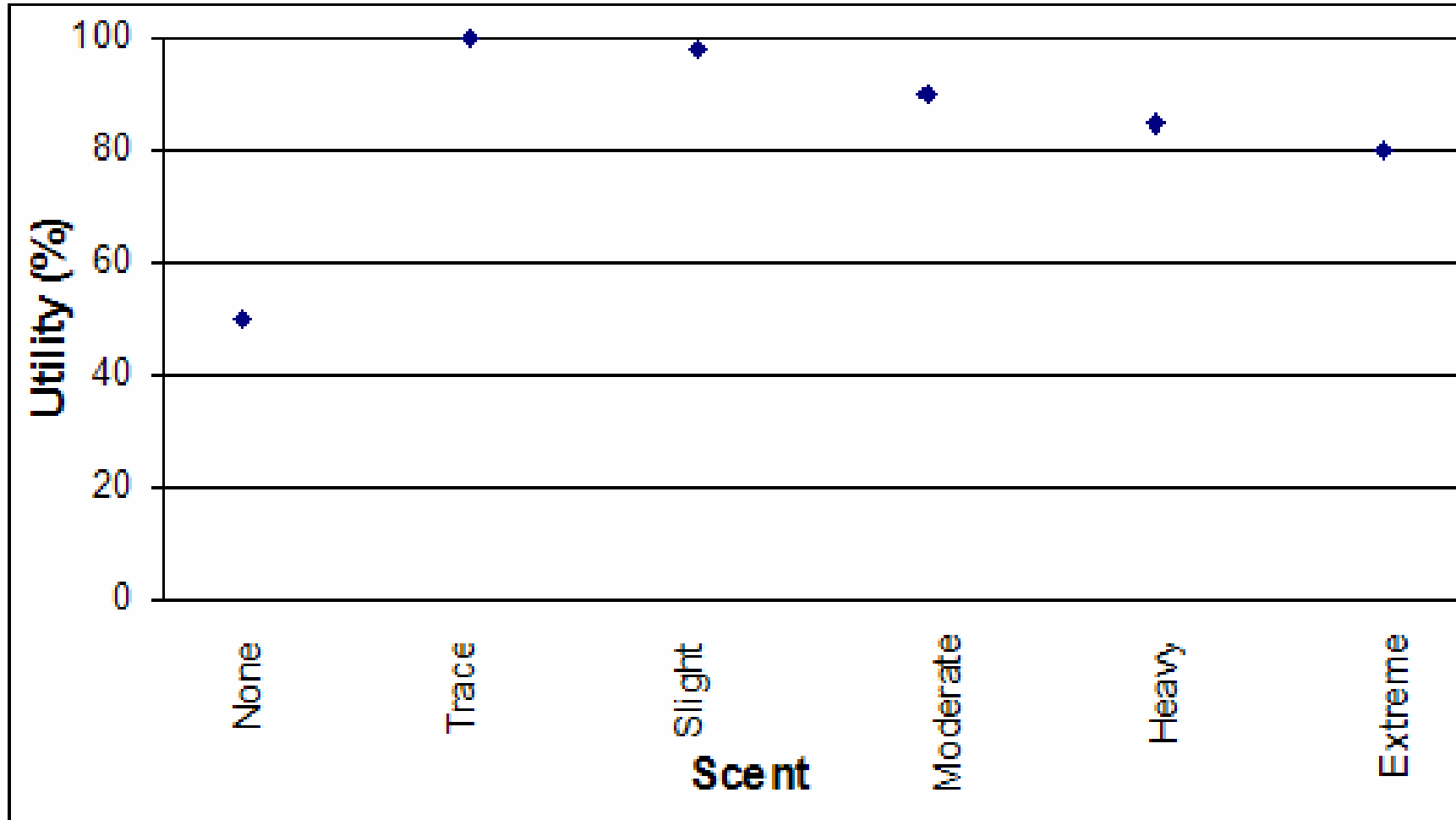


Scent Intensity relates

- Fragrance intensity
- Number of particles per unit area (n)



Scent Intensity



Quantifying Consumer Preference

- Journal of Food and Science
 - various amounts of linalool
 - human subjects determined scent intensity
 - 1.5 feet away from the sample
 - 25 minutes after the sample was prepared

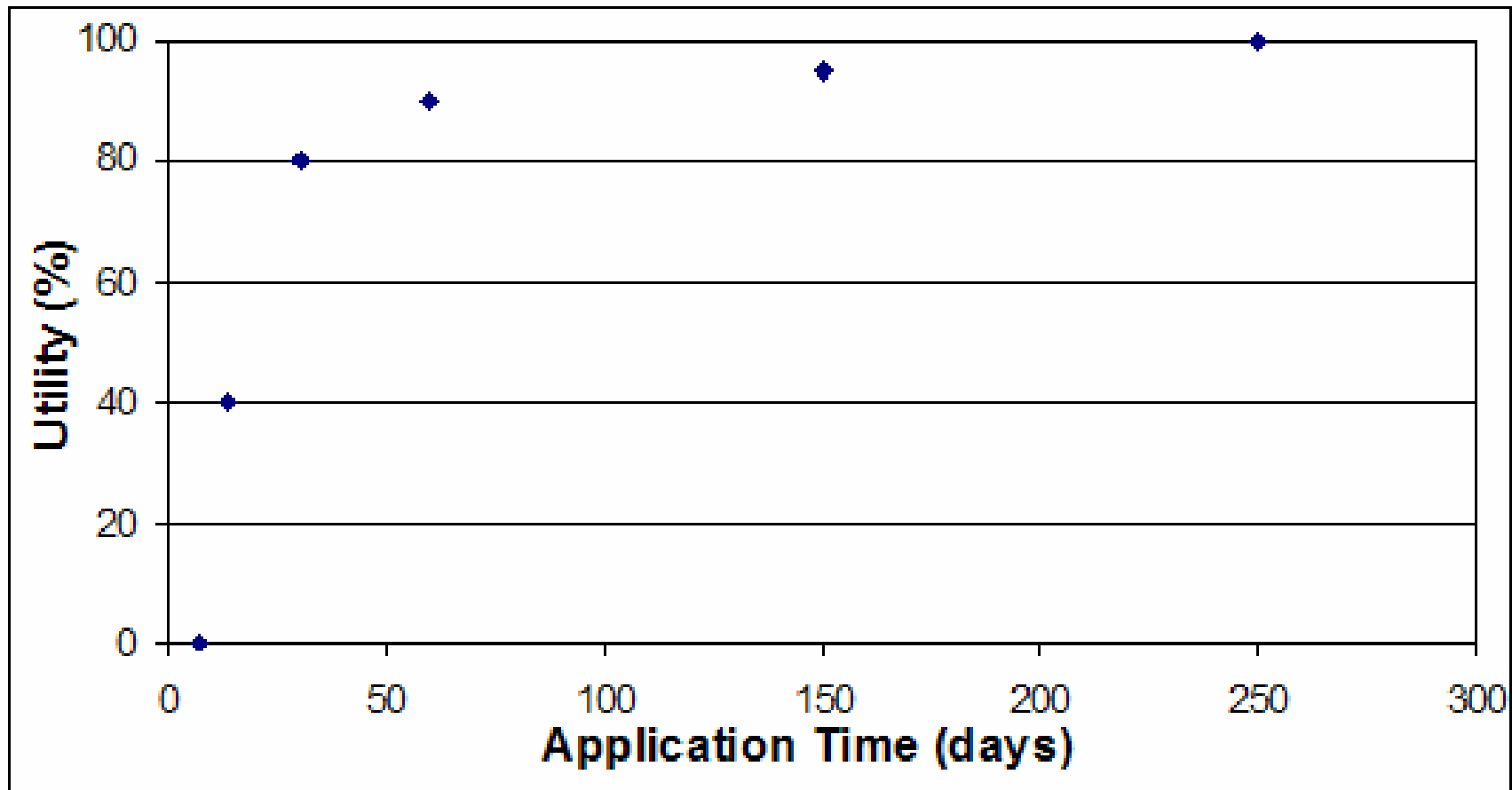
Linalool (ppm)	Strength	Utility
0	none	50
0.5	none - trace	70
2.5	trace	100
12.5	trace - slight	99
62.5	moderate	90
312.5	heavy	82.5

Fragrance Duration relates

- Application frequency
- Amount of linalool in particles (L)



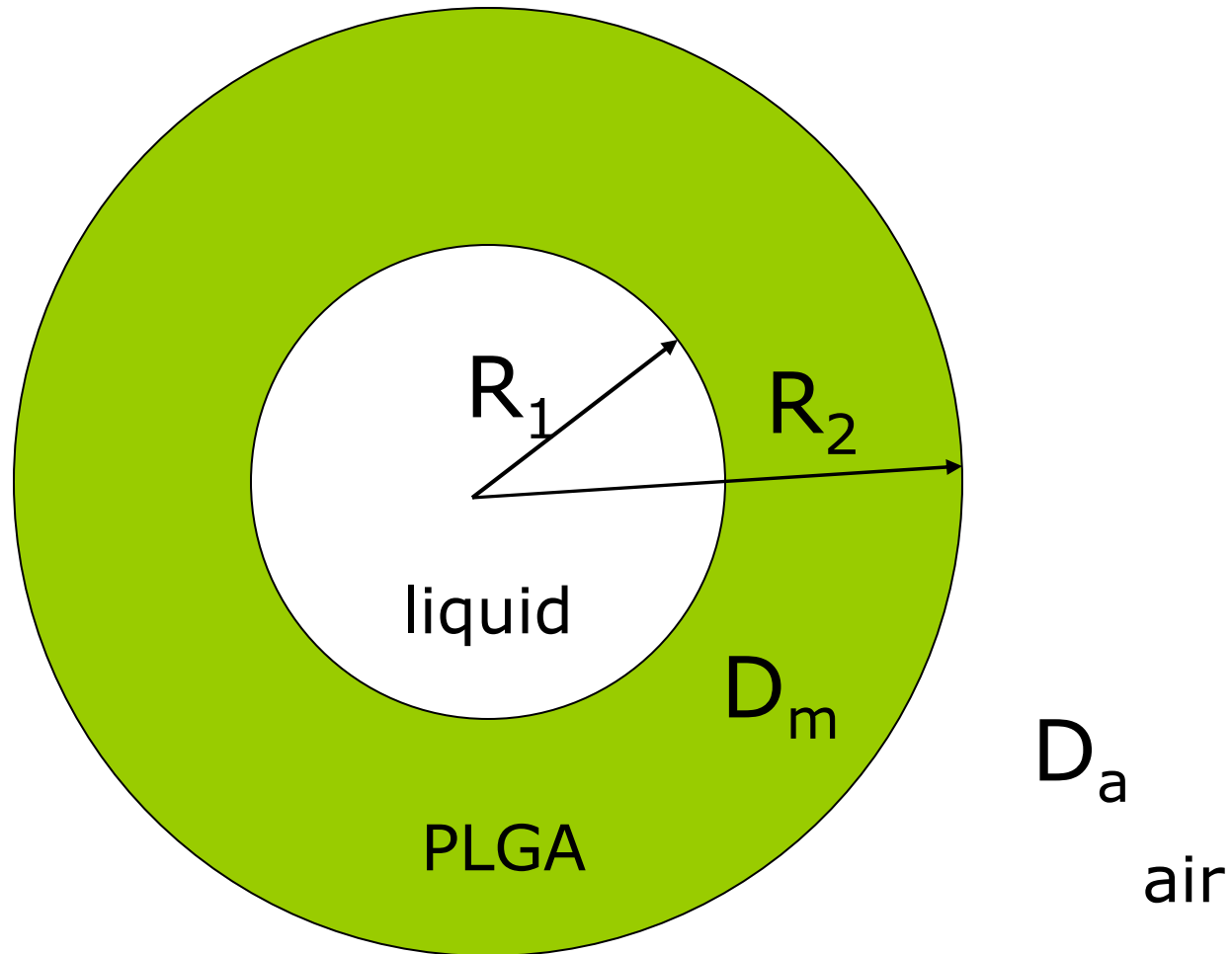
Fragrance Duration



Mass Transfer quantifies

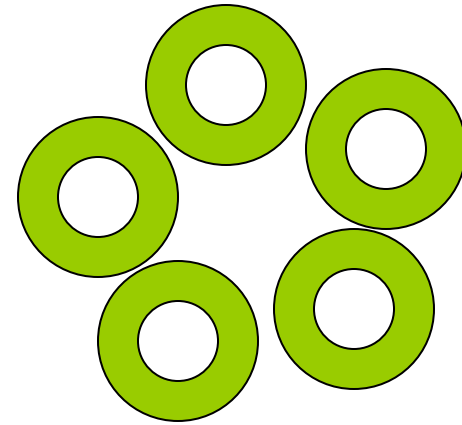
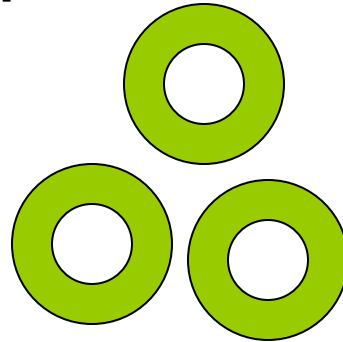
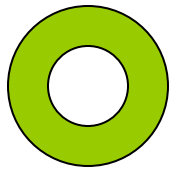
- Scent Intensity
- Fragrance Duration

Fragrance Particle Schematic



Design Parameters

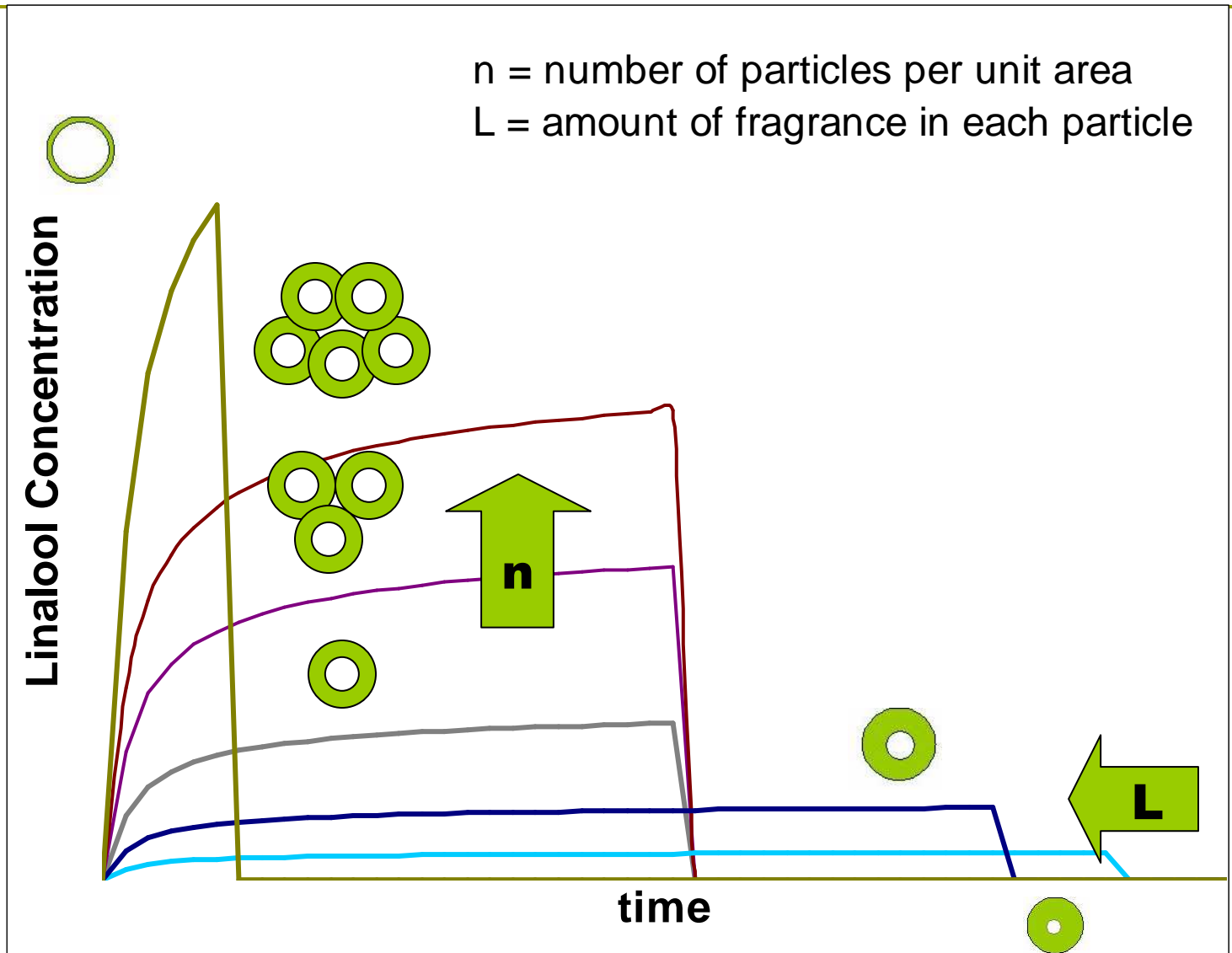
- Number of particles (n)



- Amount of linalool in particles (L)



Expected Trends

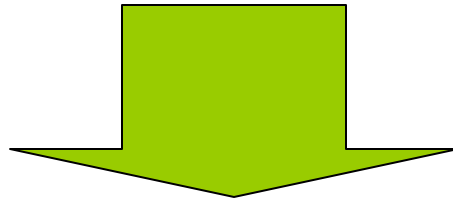


Assumptions

- Radial symmetry
- Air is semi-infinite
- No degradation inside particle
- Polymer degradation slower than fragrance diffusion

Equation Development

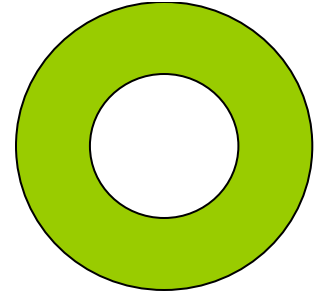
$$\frac{d}{dr} \left(r^2 \frac{dC}{dr} \right) = 0$$



$$C = b - \frac{a}{r}$$

Welty et al., "Fundamentals of Momentum, Heat, and Mass Transfer," 2001.

Boundary Conditions



$$\blacksquare C = c^{sat} \quad \text{at } r = R_1$$

$$\blacksquare D_m \frac{dC}{dr} \Big|_{r=R_2} = D_a \frac{dC^*}{dr} \Big|_{r=R_2}$$

$$\blacksquare r > R_2$$

$$C^* = C^*_{\infty} + (C^*(R_2) - C^*_{\infty}) \frac{R_2}{r} \operatorname{erfc} \left(\frac{r - R_2}{2\sqrt{D_a t}} \right)$$

Linalool Concentration

$$C(r) = c^{sat} - \frac{R_2}{R_1} \frac{D_a}{D_m} C(R_2) + \frac{R_2}{r} \frac{D_a}{D_m} C(R_2)$$

$$C(R_2) = \frac{c^{sat}}{1 + \frac{R_2}{R_1} \frac{D_a}{D_m} - \frac{D_a}{D_m}}$$

Scent Intensity

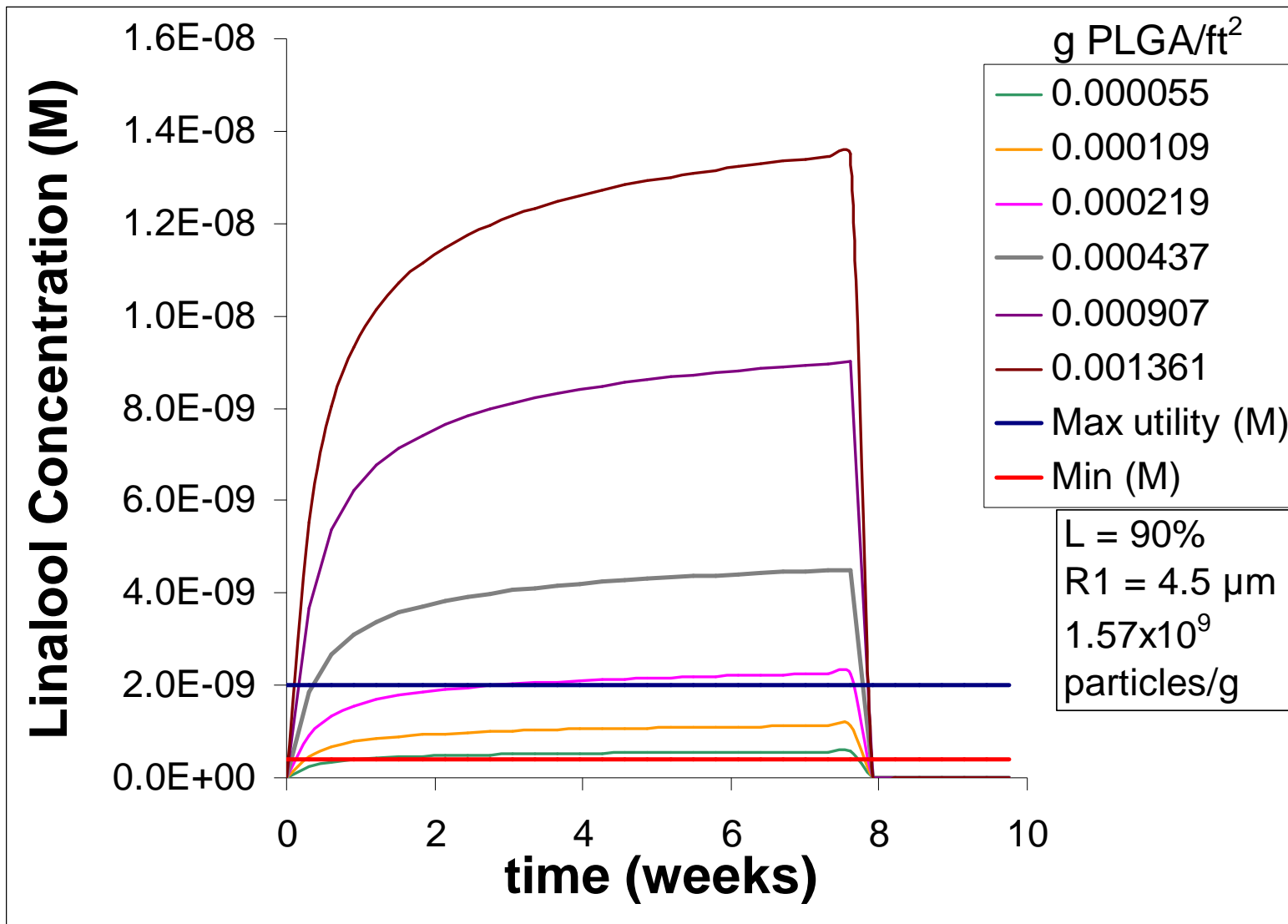
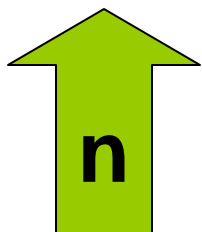
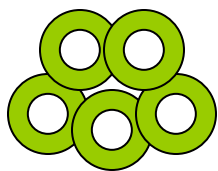
□ Relates

- Odor intensity
- Number of particles per unit area (n)

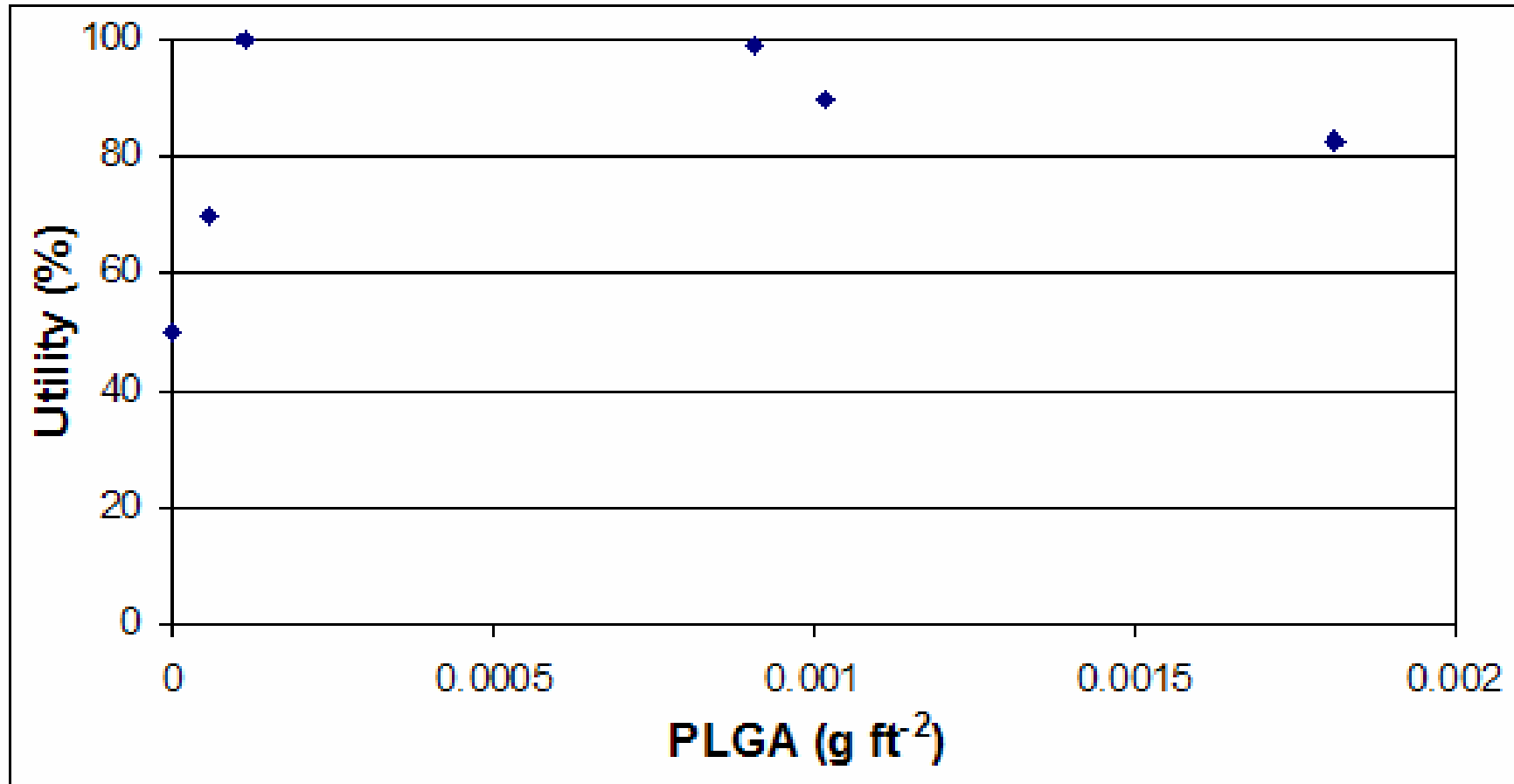
□ Assuming

- 10 micron particle diameter
- Fixed amount of linalool in particles (L) to 90% linalool

Scent Intensity: Concentration at 5 ft



Scent Intensity



Fragrance Duration

$$\int_0^{t^*} D_m \frac{dC}{dr} = m$$

$$t^* = \frac{c_o R_1^3}{3D_a C(R_2) R_2}$$

Fragrance Duration

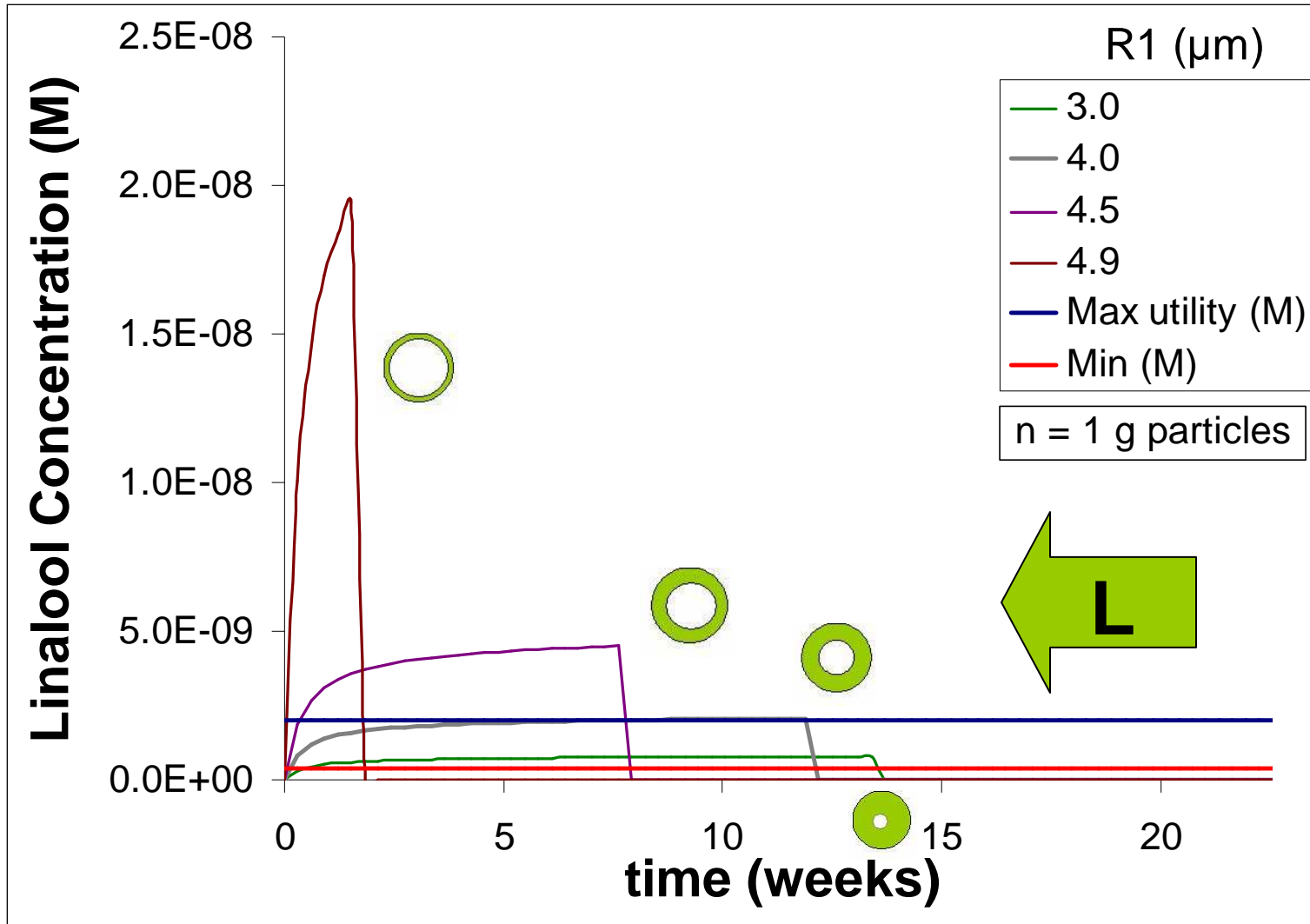
□ Relates

- Application frequency
- Amount of linalool in particles (L)

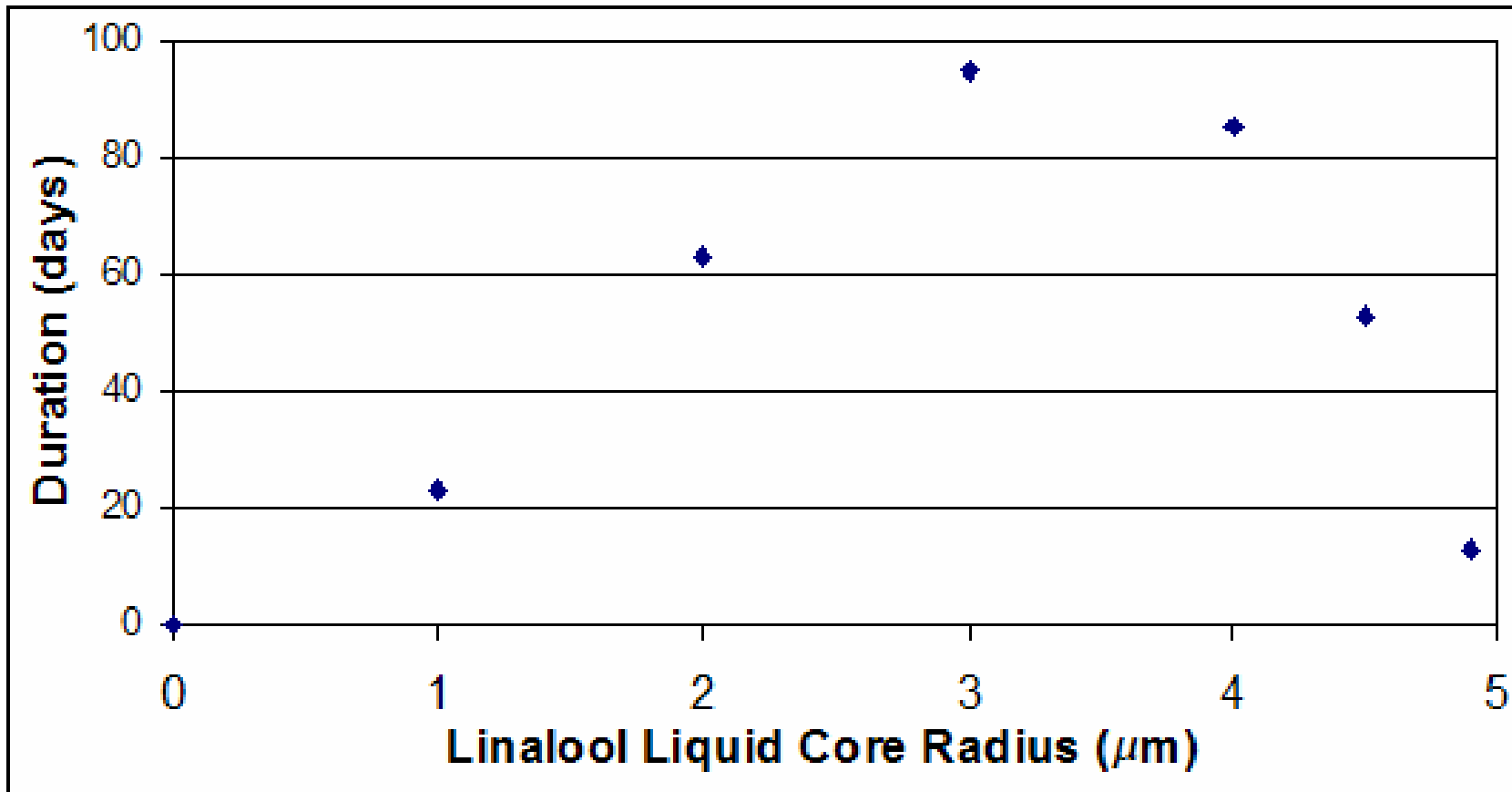
□ Assuming

- 24 hours to concentration threshold
- Fixed number of particles (n)

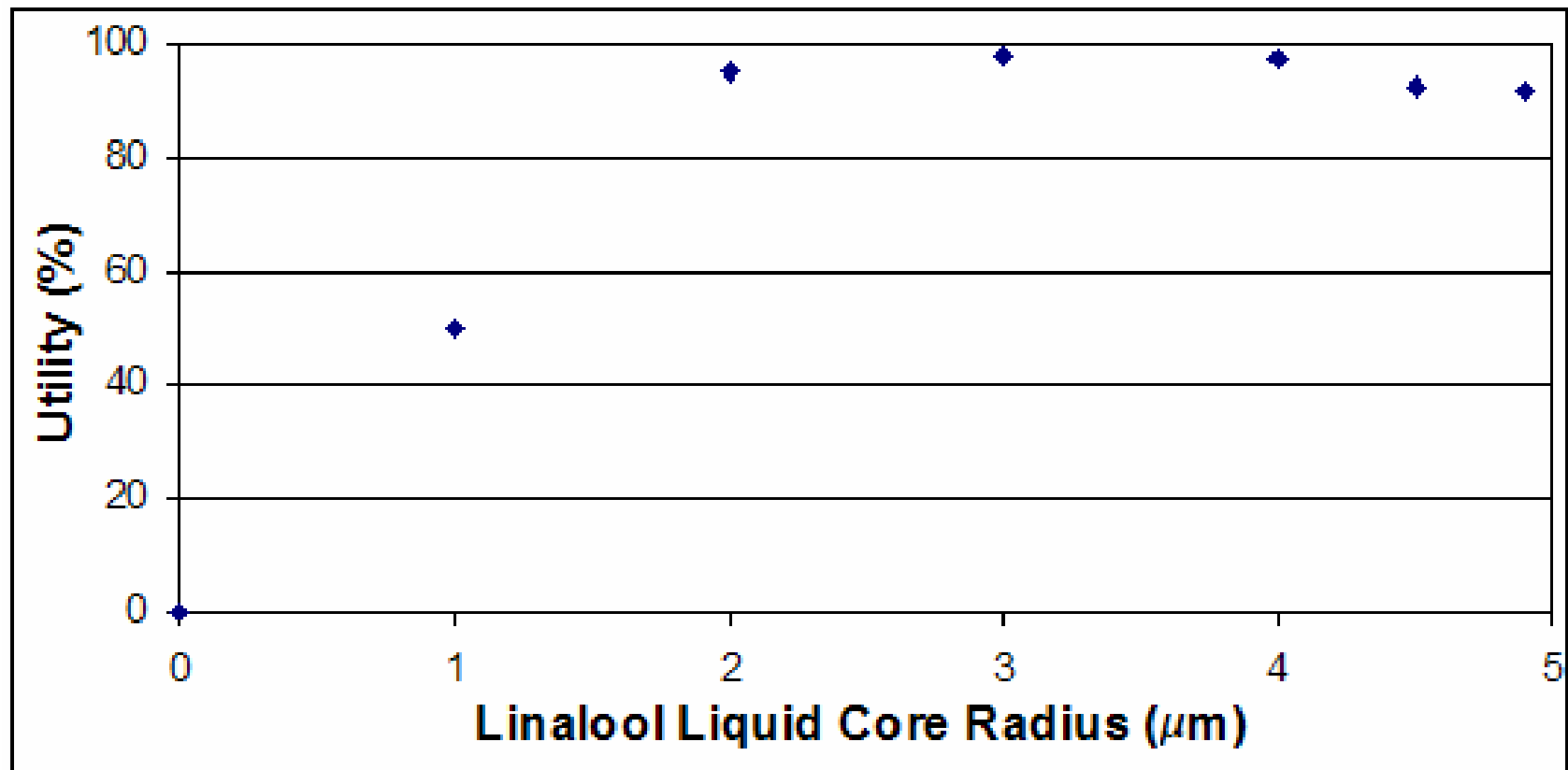
Fragrance Duration: Concentration at 5 ft



Fragrance Duration



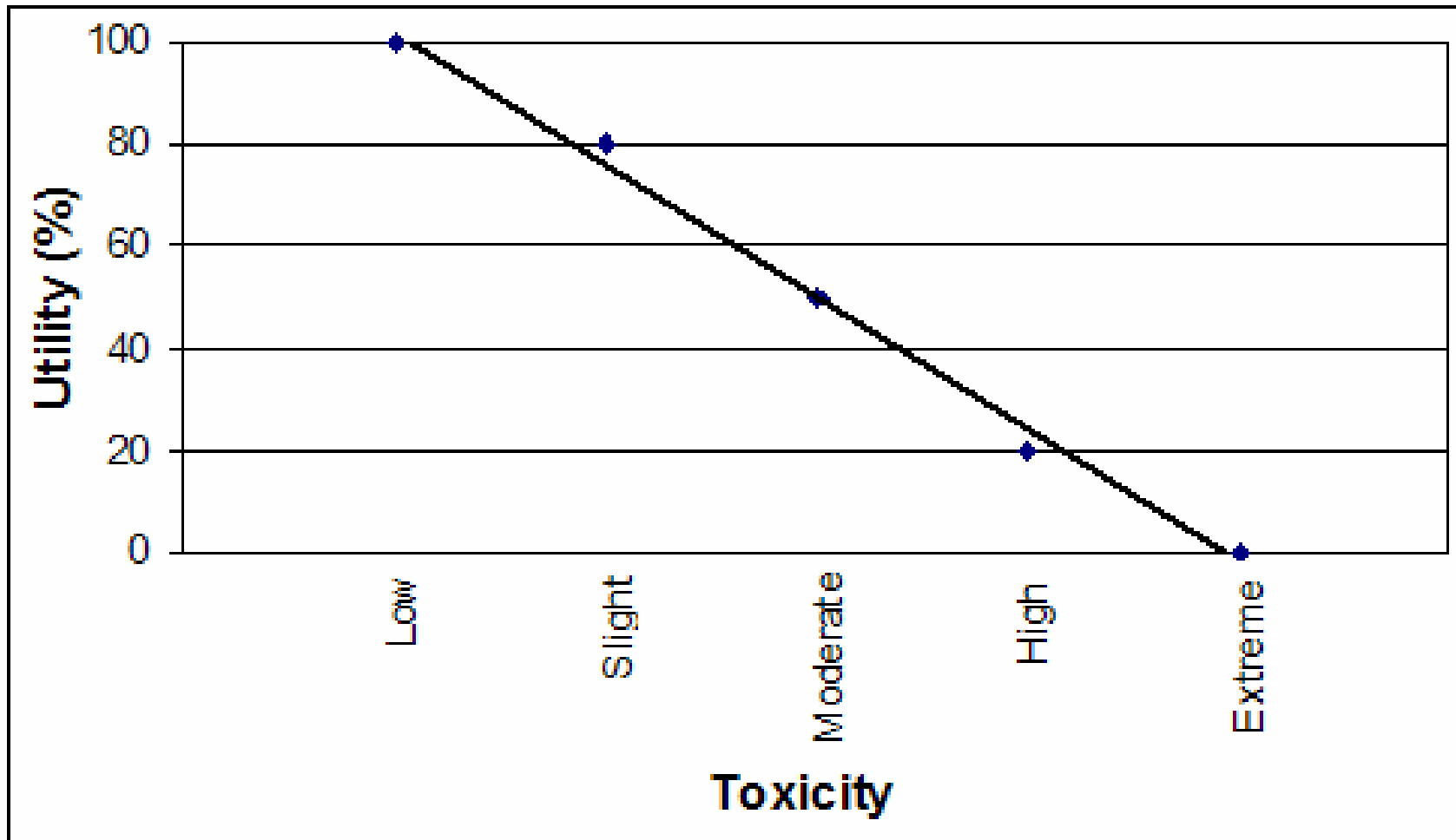
Fragrance Duration



Toxicity relates

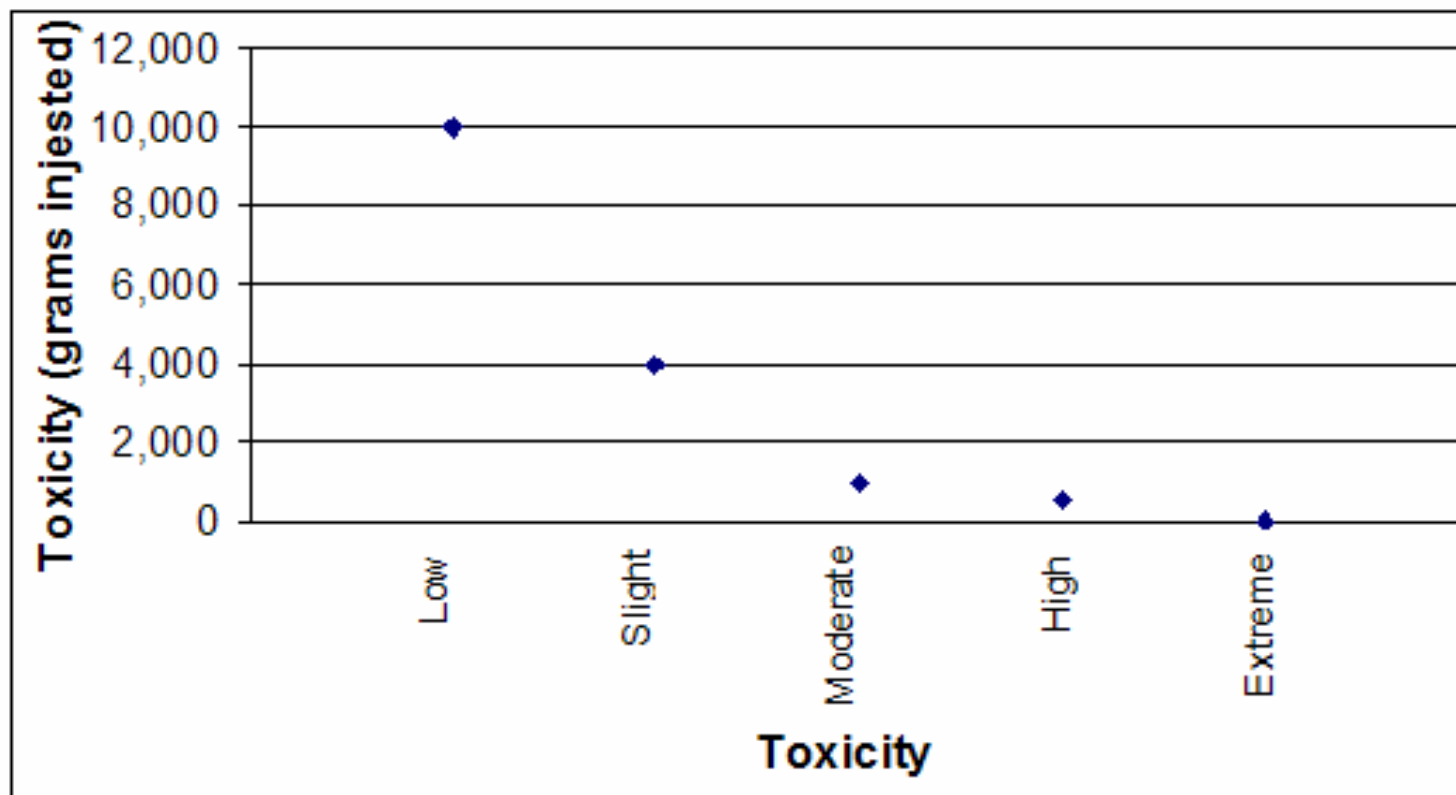
- Toxicity
- Amount of boric acid per unit area

Toxicity

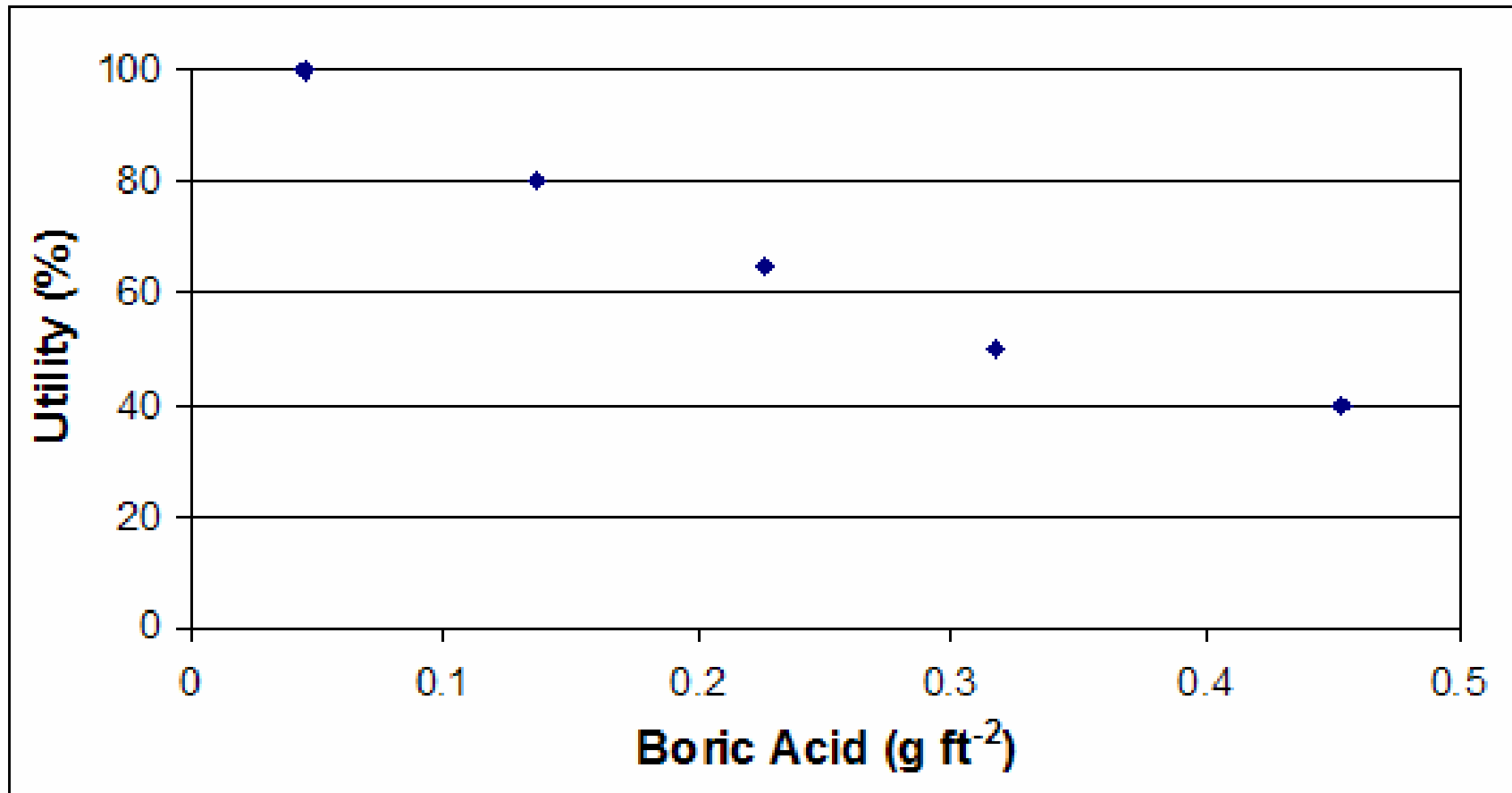


Toxicity

- Components are fixed
- Toxicity is the same as the competitor



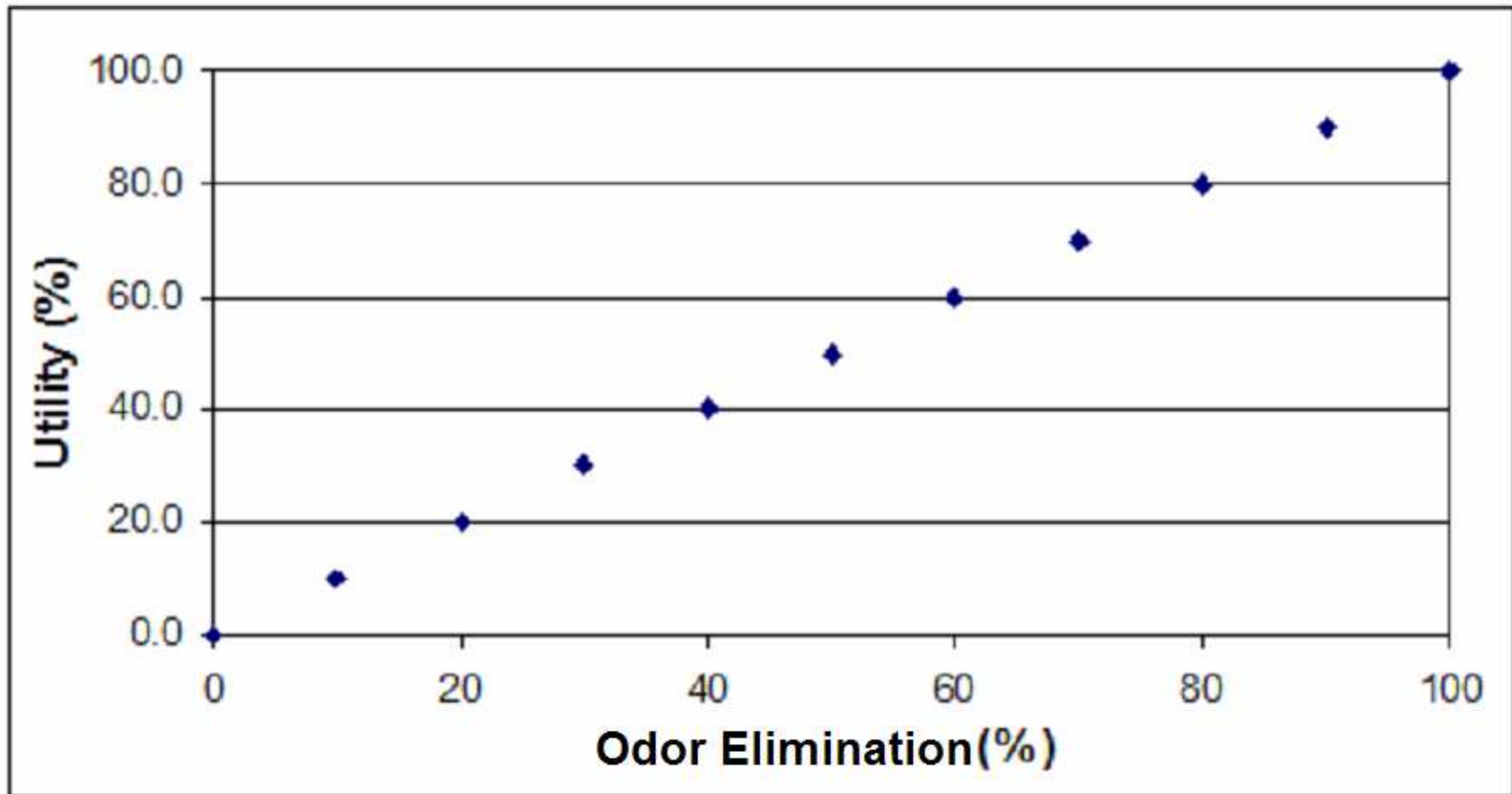
Toxicity



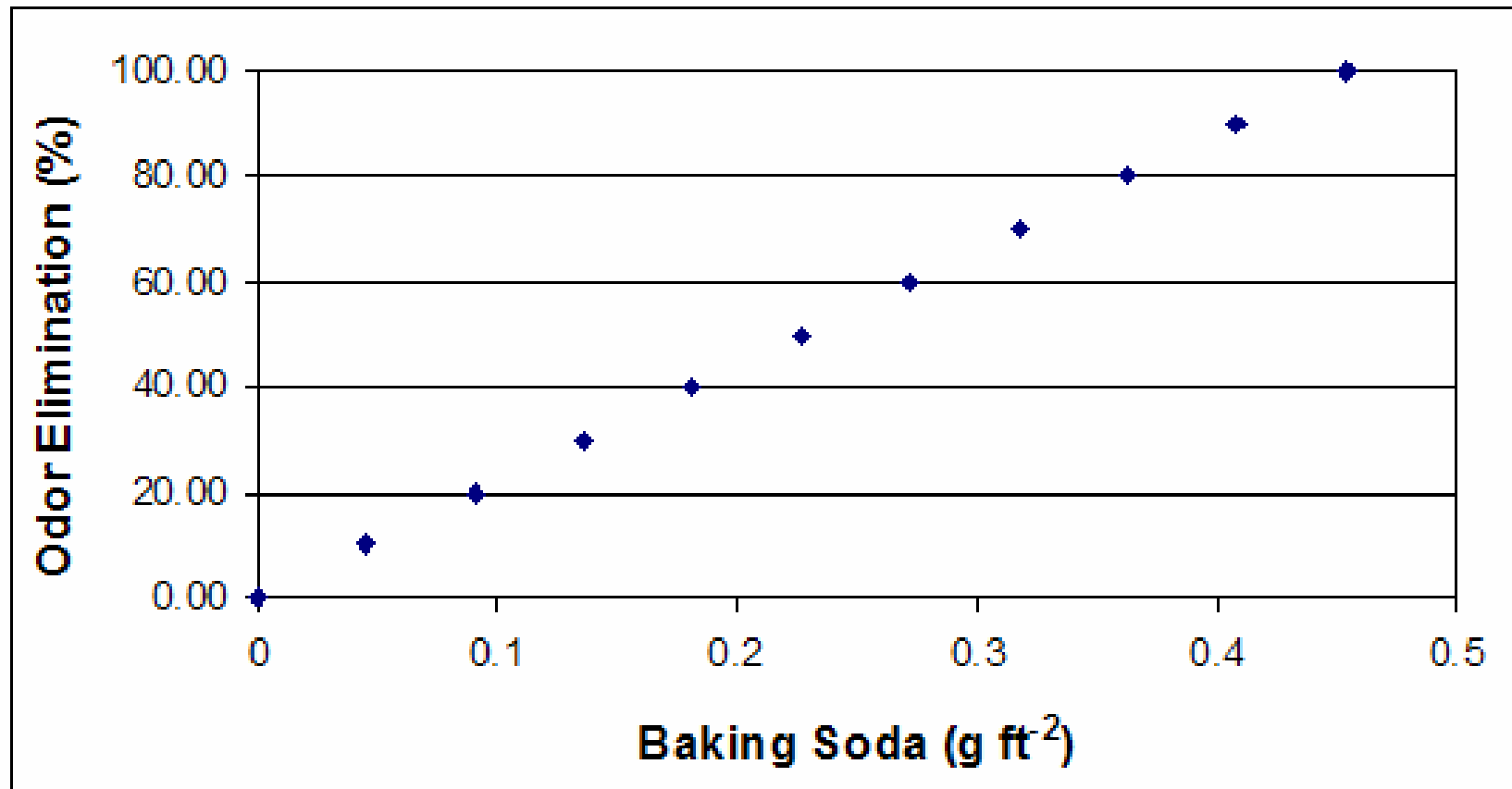
Odor Elimination relates

- Odor Eliminated (Freshness)
- Amount of baking soda per unit area

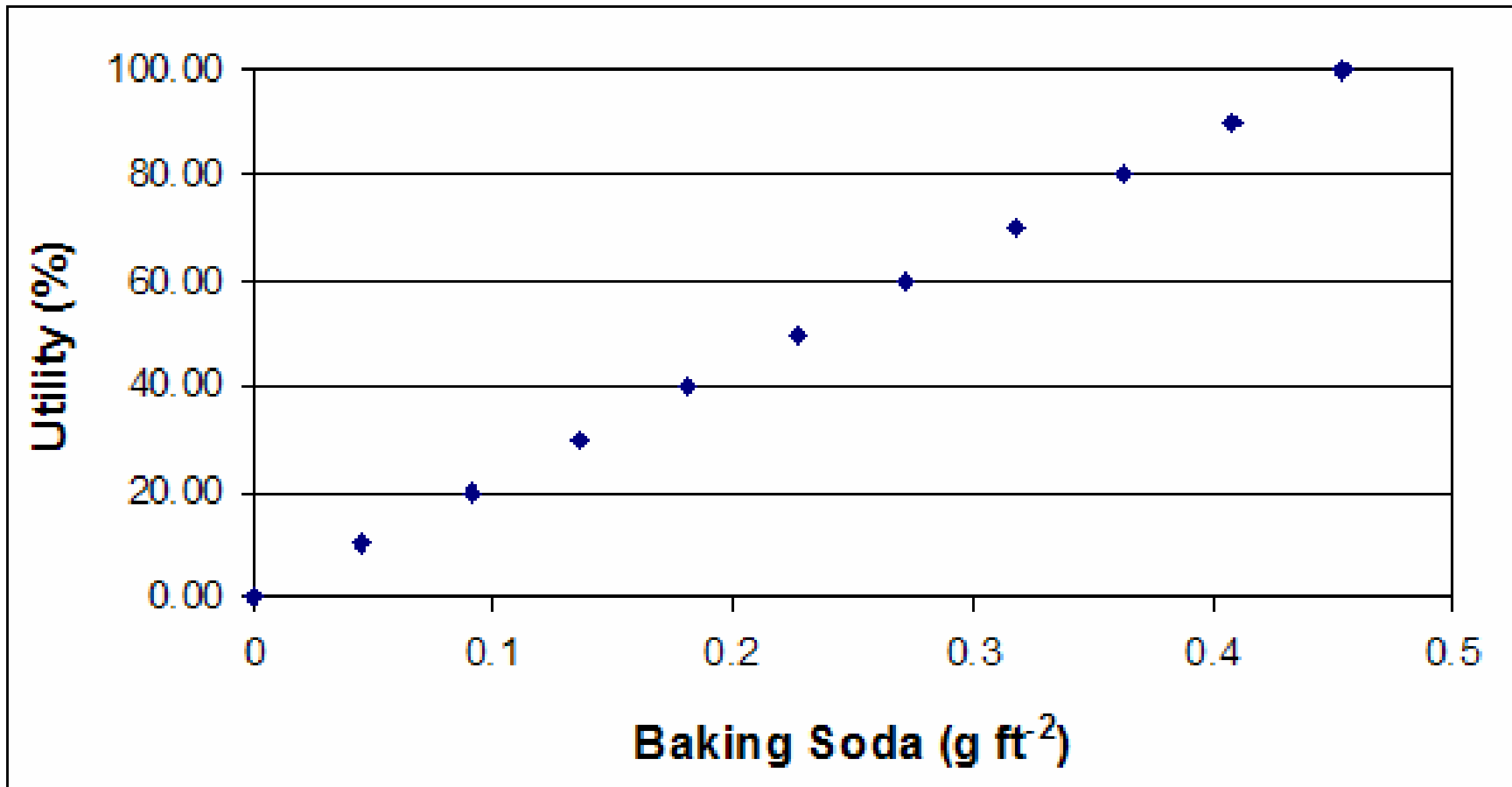
Odor Elimination



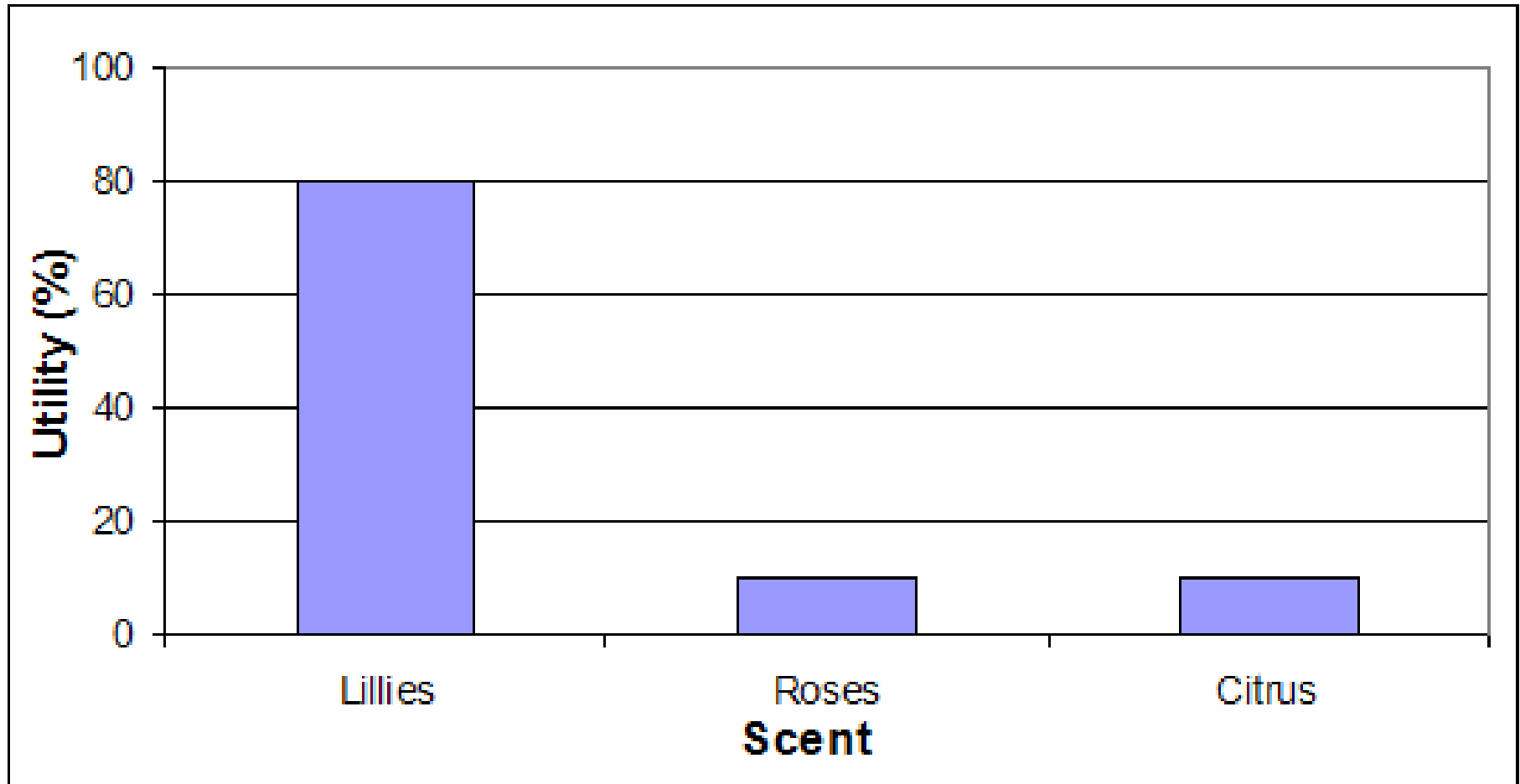
Odor Elimination



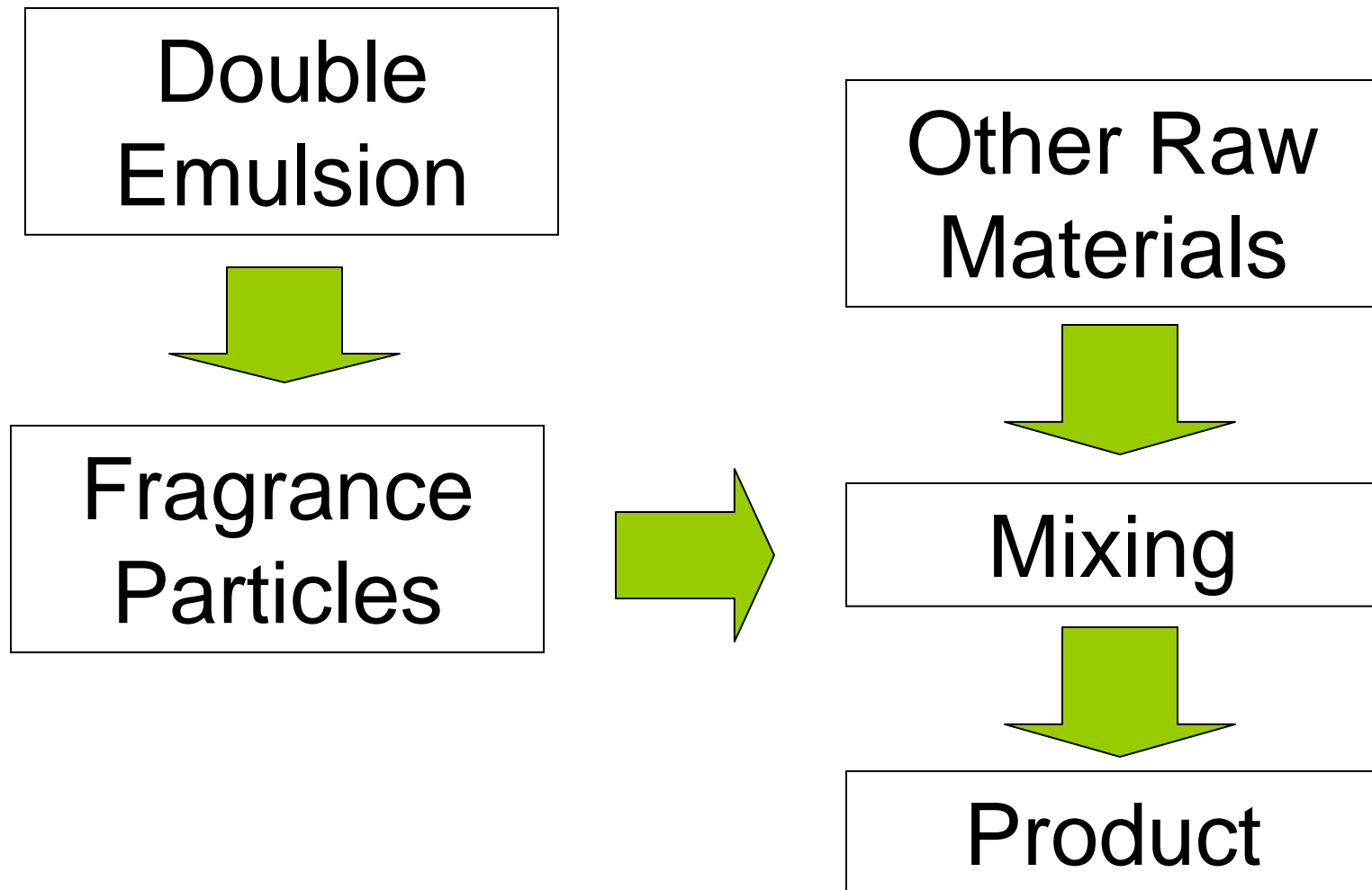
Odor Elimination



Scent Type

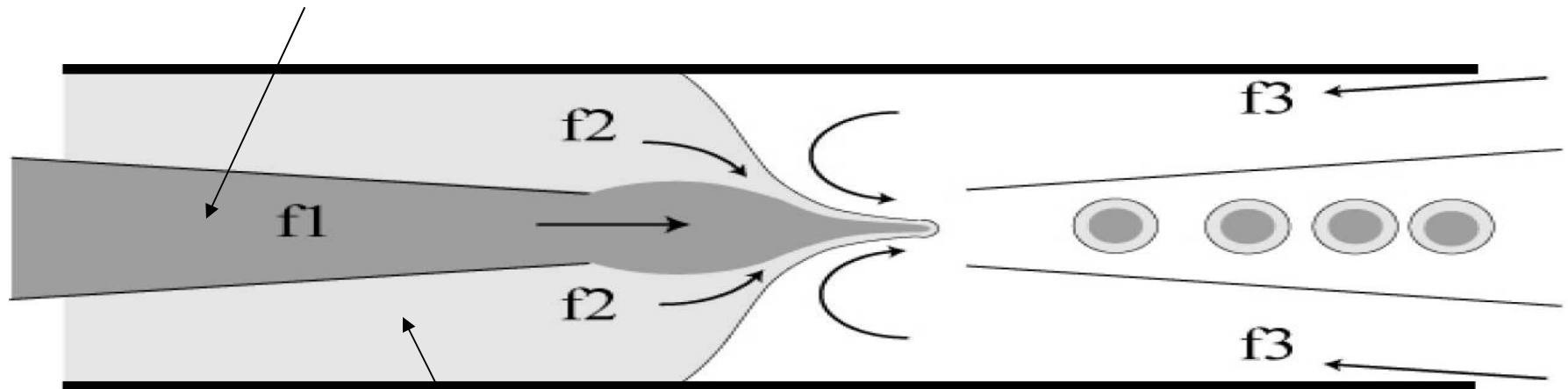


Production Process



Water/Oil/Water Double Emulsion

Aqueous linalool



Methylene
chloride/PLGA solution

Double Emulsion

- Mix by sonication

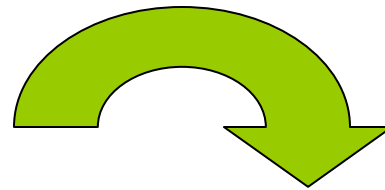


Sonicator

www.2spi.com

Double Emulsion

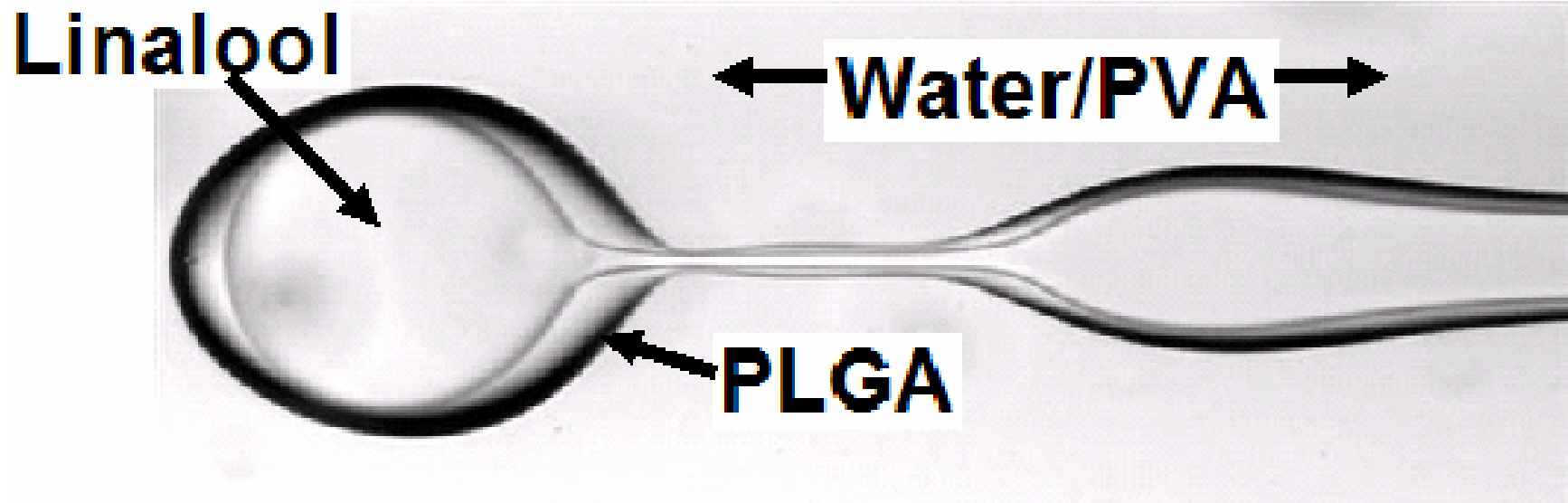
Linalool
in methylene
chloride/PLGA



H₂O and PVA
(emulsifying agent)

Double Emulsion

- PVA ensures small colloids stay small



Double Emulsion

- Remove organic solvent



Rotary Evaporator

aironline.com/equipment

Double Emulsion

- ▣ Collect microspheres



Centrifuge

aironline.com/equipment/

Double Emulsion

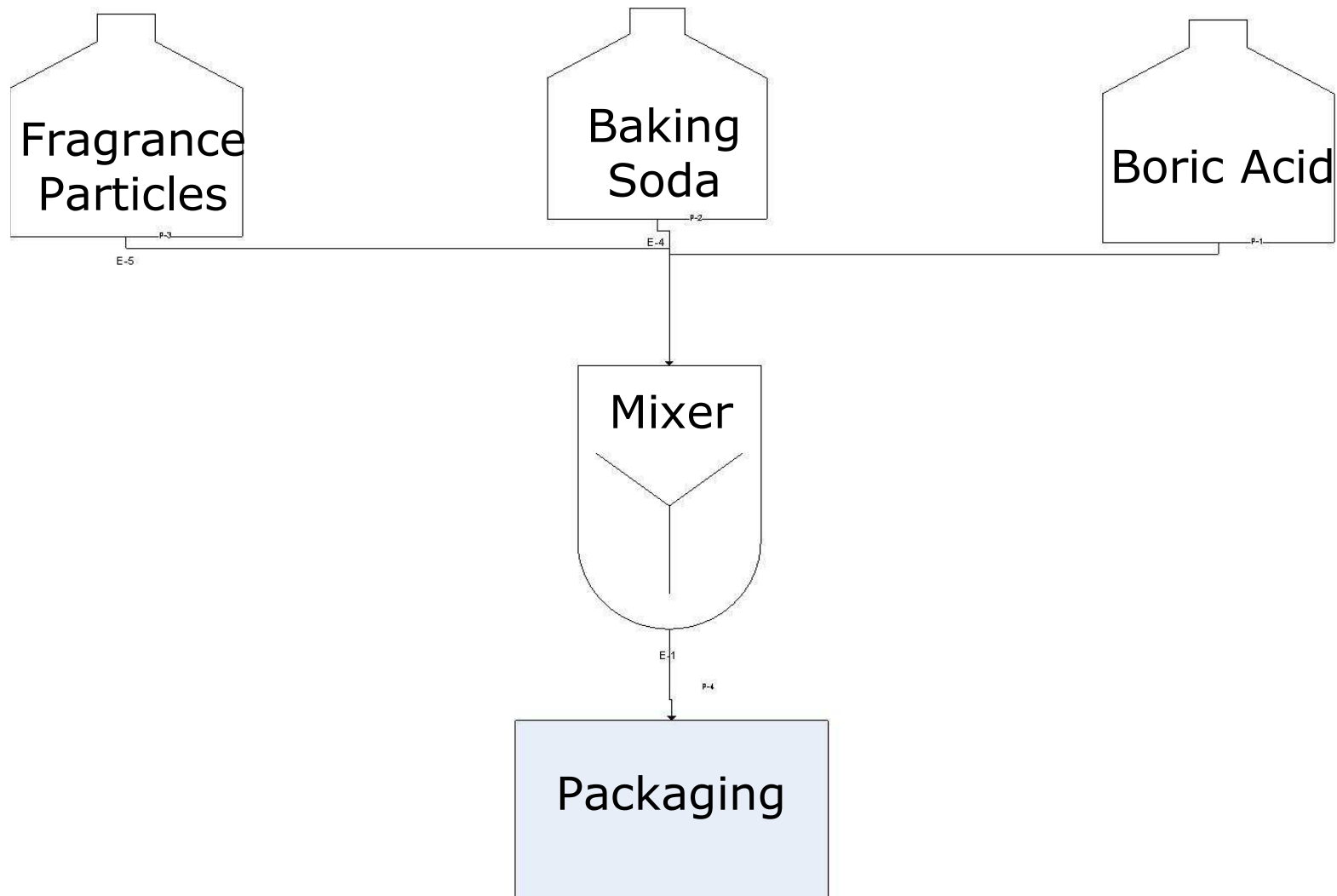
- Prepare for mixing



Freeze Dryer

www.labx.com

Production Process: Mixing



Cost Analysis

- TCI and FCI
- Price and Demand Model
 - Maximized Utility
 - Maximized NPW
- Shipping Costs
- Advertising Costs
- Risk
 - Strauss Plots
 - Monte-Carlo Simulations

Price and Demand

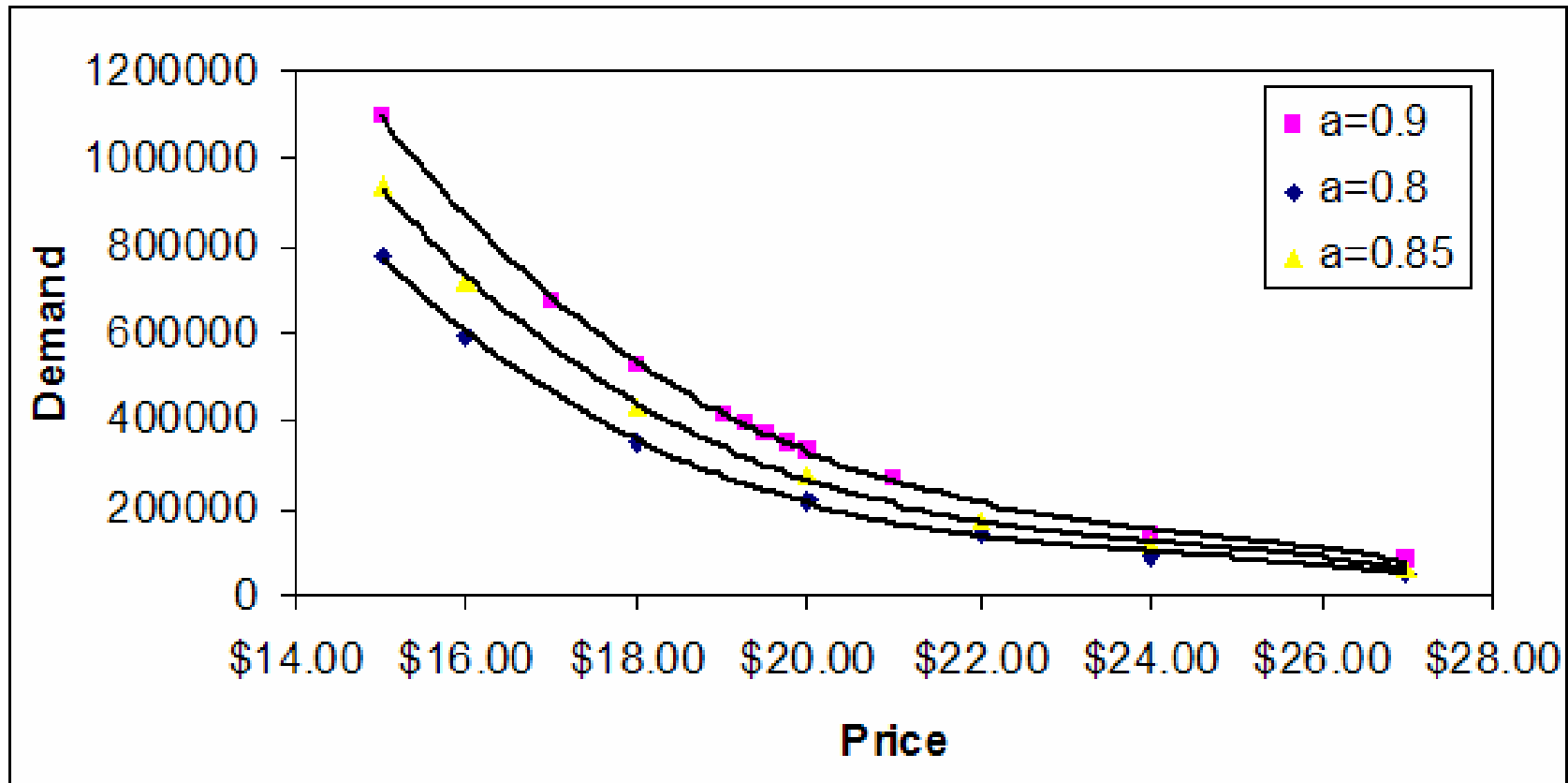
$$0 = P_1 D_1 - \left(\frac{\alpha}{\beta} \right)^\rho P_2 \left(\frac{Y - P_1 D_1}{P_2} \right)^{1-\rho} D_1^\rho$$

α	= consumer awareness
β	= competitor utility/our utility
ρ	= diminishing marginal utility (concave <1)
Y	= budget constraint
P	= price
D	= demand
	1 = ours, 2 = competition

$$P_2 = 10\$$$

$$U_2 = 62$$

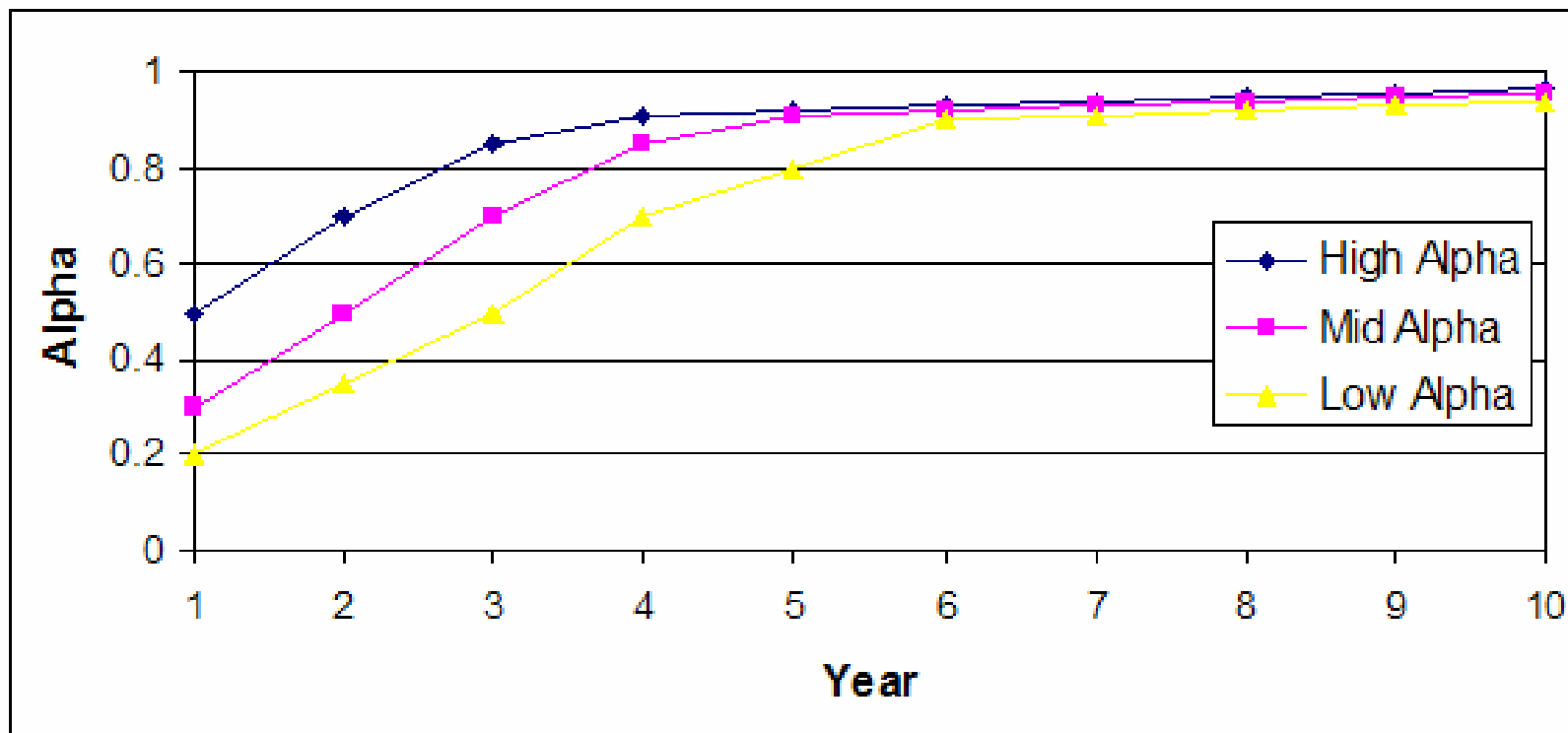
Price and Demand



Budget Constraint = 54 million

Alpha

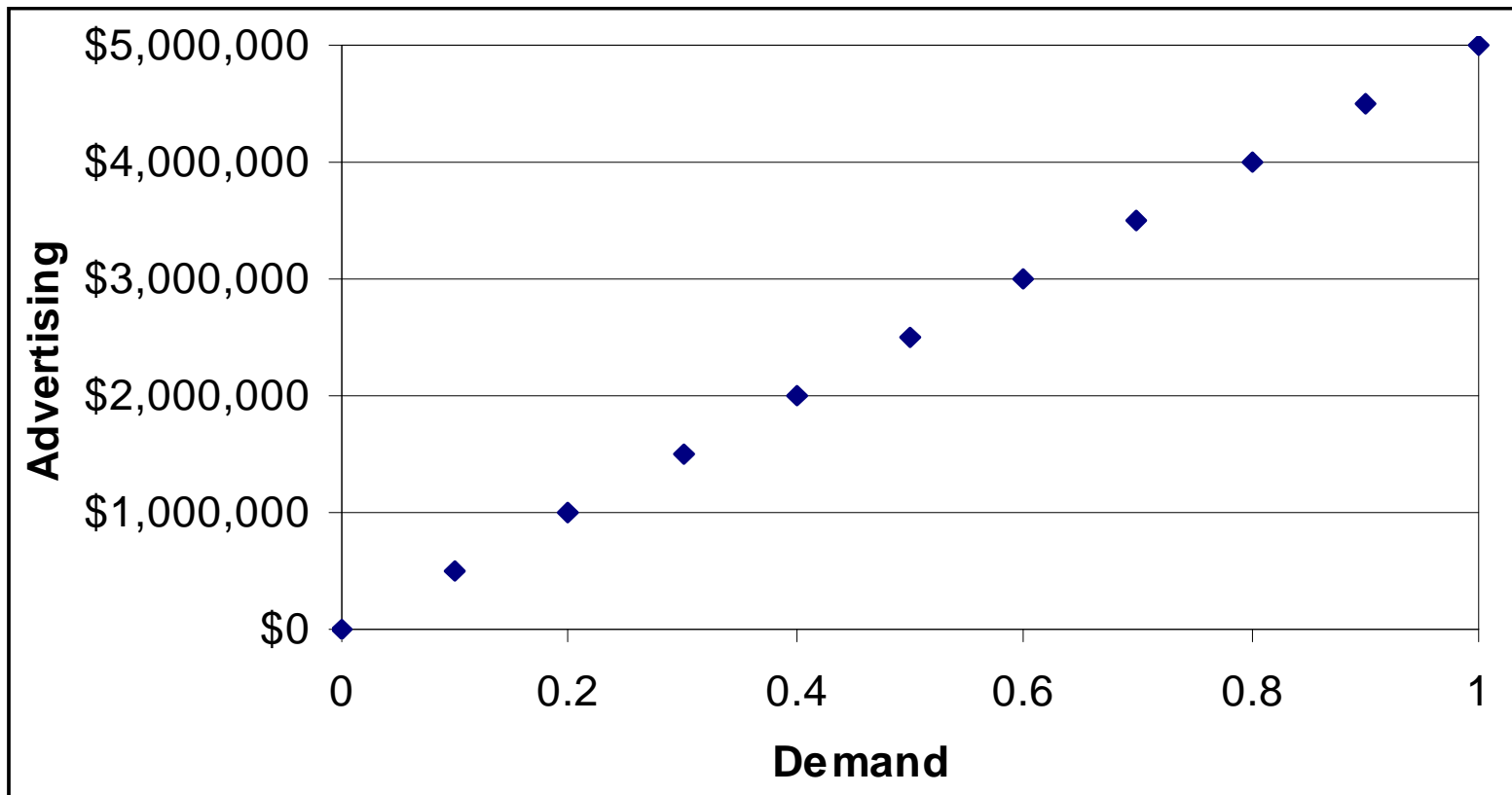
- α is a function of advertising and time



- Preliminary estimates based on $\alpha = 0.9$

Advertising

- Directly proportional to demand
- \$5 million for 100% demand



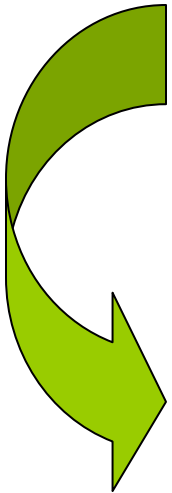
Shipping

Choose
Distribution
Centers

throughout USA

Assign
Weights

population and
humidity

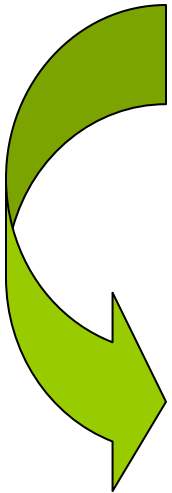


Shipping

Possible
Plant
Locations

high productivity

Minimize
Cost



Shipping Assumptions

- Ship by truck
- Constant product composition
- Uniform price in all regions
- Uniform budget constraint in all regions

Distribution Centers

Olympia, WA

Salt Lake City, UT

Denver, CO

Austin, TX

Jefferson City, MO

Indianapolis, IN

Tallahassee, FL

Albany, NY

Sacramento, CA

Phoenix, AZ

Helena, MT

Baton Rouge, LA

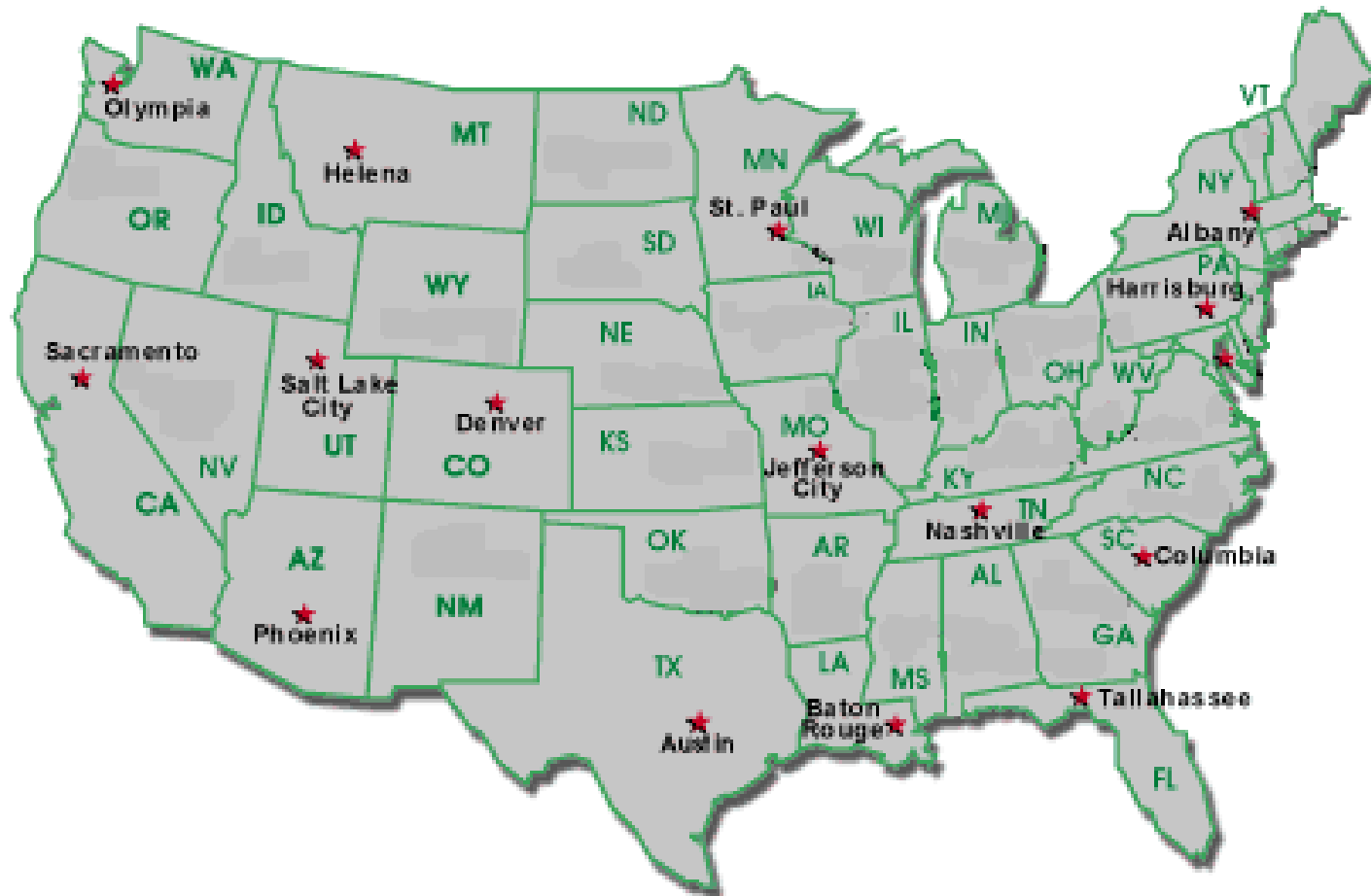
St Paul, MN

Nashville, TN

Columbia, SC

Harrisburg, PA

Distribution Centers



Shipping Calculations

Microsoft Excel - Shipping Costs

File Edit View Insert Format Tools Data Window Help

Type a question for help

75%

Arial 10 B I U

Reply with Changes... End Review...

D28 1155


	A	B	C	D	E	F	G	H	I	J	K
1											
2											
3	Distribution Center	Population			Humidity						
4	Locations	surrounding each			of each						
5	evenly distributed throughout	center			area				Population	Humidity	Percenta
6	continental US	wikipedia.org			http://www.cit				relative to	relative to	Weight
7					grating.com/r				average	average	Received
8					relativehumidi						
9					ty.asp						
10					AM	PM	Average				
11	Olympia, WA	3,919,624	3,900,000	metro (Seattle)	62%	64%	78%		2.34	1.18	1.76
12	Salt Lake City, UT	1,005,232	1,000,000	metro	67%	43%	55%		0.60	0.83	0.72
13	Denver, CO	2,330,146	2,300,000	metro	67%	40%	54%		1.39	0.81	1.10
14	Austin, TX	1,412,271	1,400,000	metro	63%	53%	71%		0.84	1.08	0.96
15	Jefferson City, MO	2,706,117	2,700,000	metro (St. Louis)	61%	63%	72%	(Kansas City, MO)	1.61	1.09	1.35
16	Indianapolis, IN	1,939,349	1,900,000	metro	84%	62%	73%		1.16	1.11	1.13
17	Tallahassee, FL	255,500	260,000	metro	90%	55%	73%		0.15	1.10	0.63
18	Albang, NY	825,875	830,000	metro	80%	58%	69%		0.49	1.05	0.77
19	Sacramento, CA	2,042,283	2,000,000	metro	83%	46%	65%		1.22	0.98	1.10
20	Phoenix, AZ	3,865,077	3,900,000	metro	50%	23%	37%		2.30	0.55	1.43
21	Helena, MT	67,636	68,000	metro	66%	44%	55%	(Billings, MT)	0.04	0.83	0.44
22	Baton Rouge, LA	751,965	750,000	metro	83%	62%	76%		0.45	1.15	0.80
23	St Paul, MN	2,968,805	3,000,000	metro	83%	62%	73%	(St Cloud, MN)	1.77	1.10	1.43
24	Nashville, TN	1,422,544	1,400,000	metro	83%	60%	72%		0.85	1.08	0.97
25	Columbia, SC	689,878	690,000	metro	83%	56%	70%	(Charleston, SC)	0.41	1.05	0.73
26	Harrisburg, PA	643,820	640,000	metro	76%	55%	66%	(Philadelphia, PA)	0.38	0.99	0.69
27	Average	1,677,893	1,700,000				Average	66%			Sum
28											
29											
30	Distribution Centers	Olympia, WA	Salt Lake City, UT	Denver, CO	Austin, TX	Jefferson City, MO	Indianapolis	Tallahassee, FL	Albang, NY	Sacramento, CA	Phoenix, AZ
31	Possible Plant Locations	Distances (miles)									
32	Montgomery, AL	2169	1531	1155	631	543	514	177	986	2014	1494
33	Jackson, MS	1994	1994	966	467	446	563	372	1145	1803	1269
34	Atlanta, GA	2195	1581	1202	816	545	427	229	842	2079	1586
35	Little Rock, AR	1793	1146	771	438	266	489	554	1138	1629	1129
36	Oklahoma City, OK	1532	864	500	357	364	689	841	1361	1335	838
37											
38	Distribution Centers	Olympia, WA	Salt Lake City, UT	Denver, CO	Austin, TX	Jefferson City, MO	Indianapolis	Tallahassee, FL	Albang, NY	Sacramento, CA	Phoenix, AZ
39				79.8							

Shipping Costs

Draw AutoShapes

Ready NUM

start Remote Desktop Web... Microsoft Excel - Ship... 8:20 PM



Plant Location	Population	Avg. Humidity	Fraction of Production
Olympia, WA	3.9 million	78%	0.11
St. Paul, MN	3 million	73%	0.09
Baton Rouge, LA	750,000	76%	0.05

Plant Location

Cost per gal

Montgomery, AL

\$ 304

Jackson, MS

\$ 289

Atlanta, GA

\$ 304

Little Rock, AR

\$ 260

Oklahoma City, OK

\$ 250

TCI Calculations

Microsoft Excel - utility3

File Edit View Insert Format Tools Data Window Help

75%

Reply with Changes... End Review...

D38

Equipment Costs				
Unit	Capacity	Cost(2002)	Cost(2007)	
solids storage	2547 PT&V		\$1,500.00	
sonicator	4.844617056	http://www.2spi.com/catalog/misc_lab/	\$5,000.00	
foto vap	4.844617056	http://aironline.com/equipment/category/	\$3,200.00	
centrifuge	4.844617056	http://www.labessentials.com/centrifuge/	\$1,400.00	
freeze dryer	4.844617056	http://www.labs.com/v2/newad.cfm?cat/	\$1,800.00	
mixer	2547 PT&V		\$36,940.00	
Total Equ't Cost			\$50,000.00	

Capital Investment			Raw Materials				
Direct Costs	% of Purchased Equ't		(lbs/year)	\$/lb	\$	Year 1 \$cost	
Purchased Equipment Delivered	1	\$50,000.00	Linalool	112.08	16	1793.337	1793.33714
Purchased-equipment installation	0.47	\$23,500.00					
Instrumentation and Controls	0.36	\$18,000.00	PLGA	243.66	5300	1291398	1614247.09
Piping	0.68	\$34,000.00					
Electrical Systems	0.11	\$5,500.00	Boric Acid	200542	2.2	441192.9	561491.145
Buildings	0.18	\$9,000.00					
Yard Improvements	0.1	\$5,000.00	Baking Soda	921978	0.85	783681.1	979601.376
Service facilities	0.7	\$35,000.00					
Total Direct Plant Cost		\$180,000.00	PVA (emul agent)	1218.3	1.41	1717.803	2147.2532
Indirect Costs			Methylene Chlorid	561.43	0.43	241.4142	301.76778
Engineering and Supervision	0.33	\$16,500.00	Operating Labor				170769.3
Construction Expenses	0.41	\$20,500.00	Operating Supervision		0.15	of operating la	25615.395
Legal expenses	0.04	\$2,000.00	Utilities				
Contractor's fee	0.22	\$11,000.00	Electricity	45393	0.045		2063.69734
Contingency	0.44	\$22,000.00	Maintenance		0.07	of FCI	17640
Total Indirect Plant Cost		\$72,000.00	Operating Supplies		0.15	of maintenanc	2646
			Laboratory Charges		0.15	operating labo	25615.395
Fixed Capital Investment		\$252,000.00	Taxes (property)		0.02	of FCI	5040
Working Capital		\$126,000.00	Insurance		0.01	of FCI	2520
Total Capital Investment		\$378,000.00	Rent				
			Depreciation				1220

Purchased Equipment / Total Product Cost / Utility Poll Budget / Cash Flow / Utility Con

Ready NUM

start WWS5 started on 3/7... Remote Desktop Web... utility3 utility2 6:03 PM

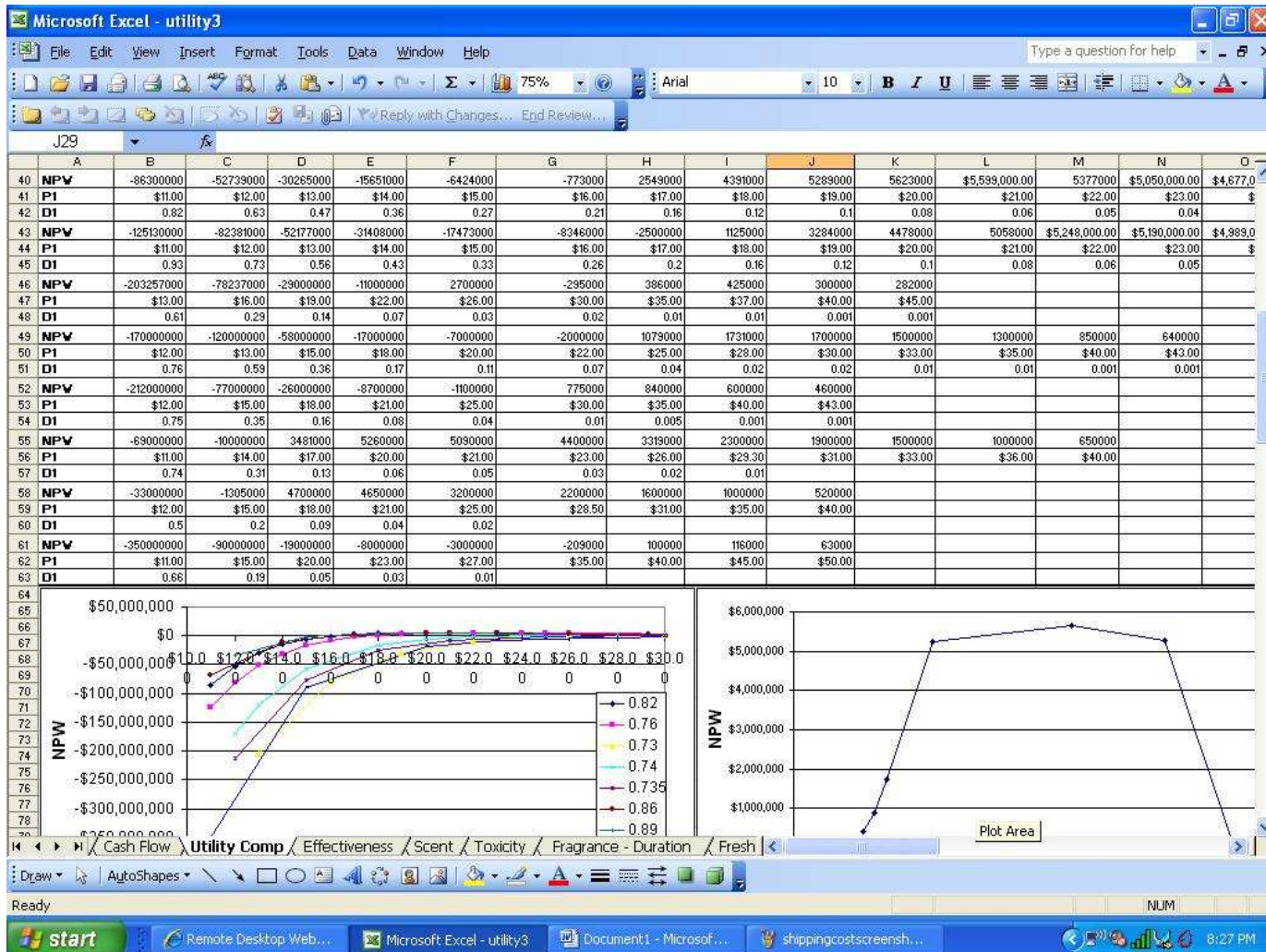
TCI Calculations

FCI	\$350,000
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Working Capital	\$175,000
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TCI	\$525,000
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NPW Calculations



Maximum Utility

□ Composition

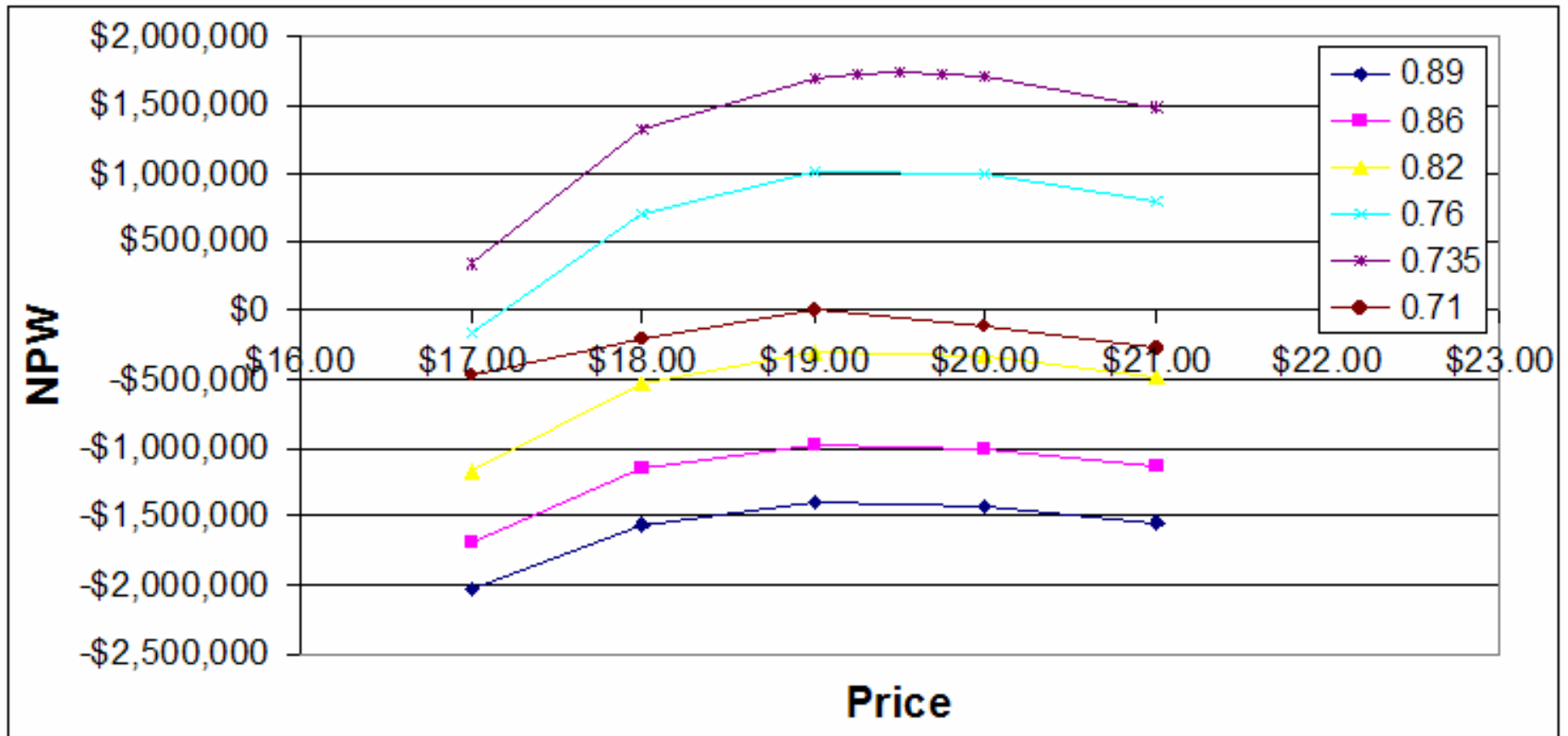
- 0.1% Linalool
- 0.2% PLGA
- 20.6% Boric Acid
- 79.1% Baking Soda

□ Cost per 16 oz container to have + NPW

- Unrealistic, you get a -NPW at any price

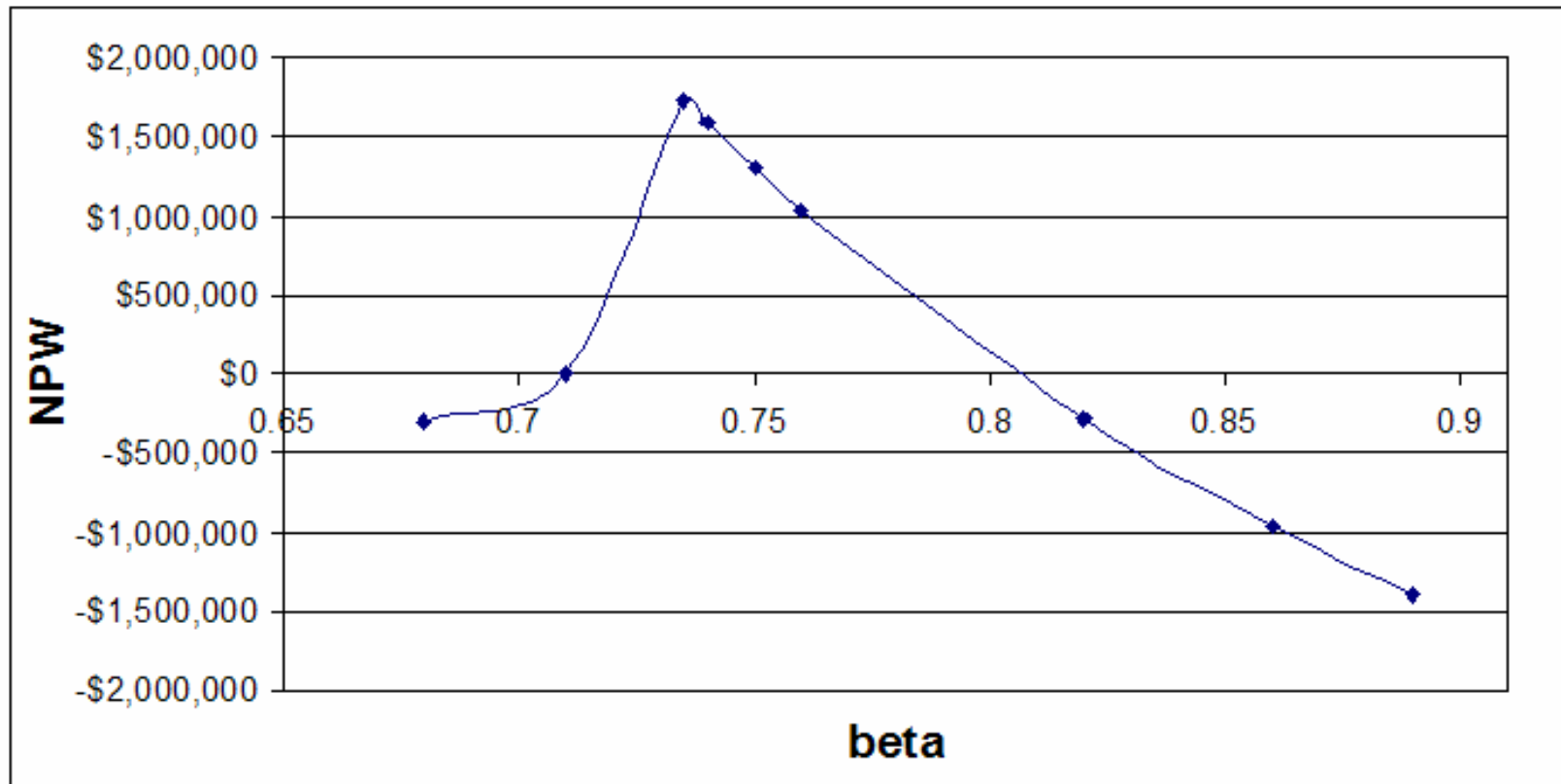
Maximum NPW Product

- Varied Composition – which varied utility



Maximum NPW Product

- Maximum NPW Utility $\beta = 0.735$ Price=\$19.44



- Composition – 0.01% Linalool, 0.02% PLGA, 17.9% Boric Acid, 80% Baking Soda

Revised Budget Constraint

- All calculations have been based on disinfectant market only
- Y=54 million
 - Max NPW is \$1,730,000 – lowest approximation
- If the air freshener market (98 million) is taken into account
 - Max NPW is \$13,300,000 – highest approximation
- Actual budget constraint most likely would fall in the middle
 - A novel idea is to poll consumers
 - How much would they pay extra than just disinfectant
 - Shown below

16oz - 10\$ container	
2x Duration	\$2.14
More Effective	\$2.03
Fresher	\$1.58
Safer	\$1.23
Better Scent	\$1.01
Increase	\$17.99
Initial Demand	5400000
New Budget Constraint	\$97,000,000.00

New Y=97 million

Max NPW = \$6,800,000

Risk

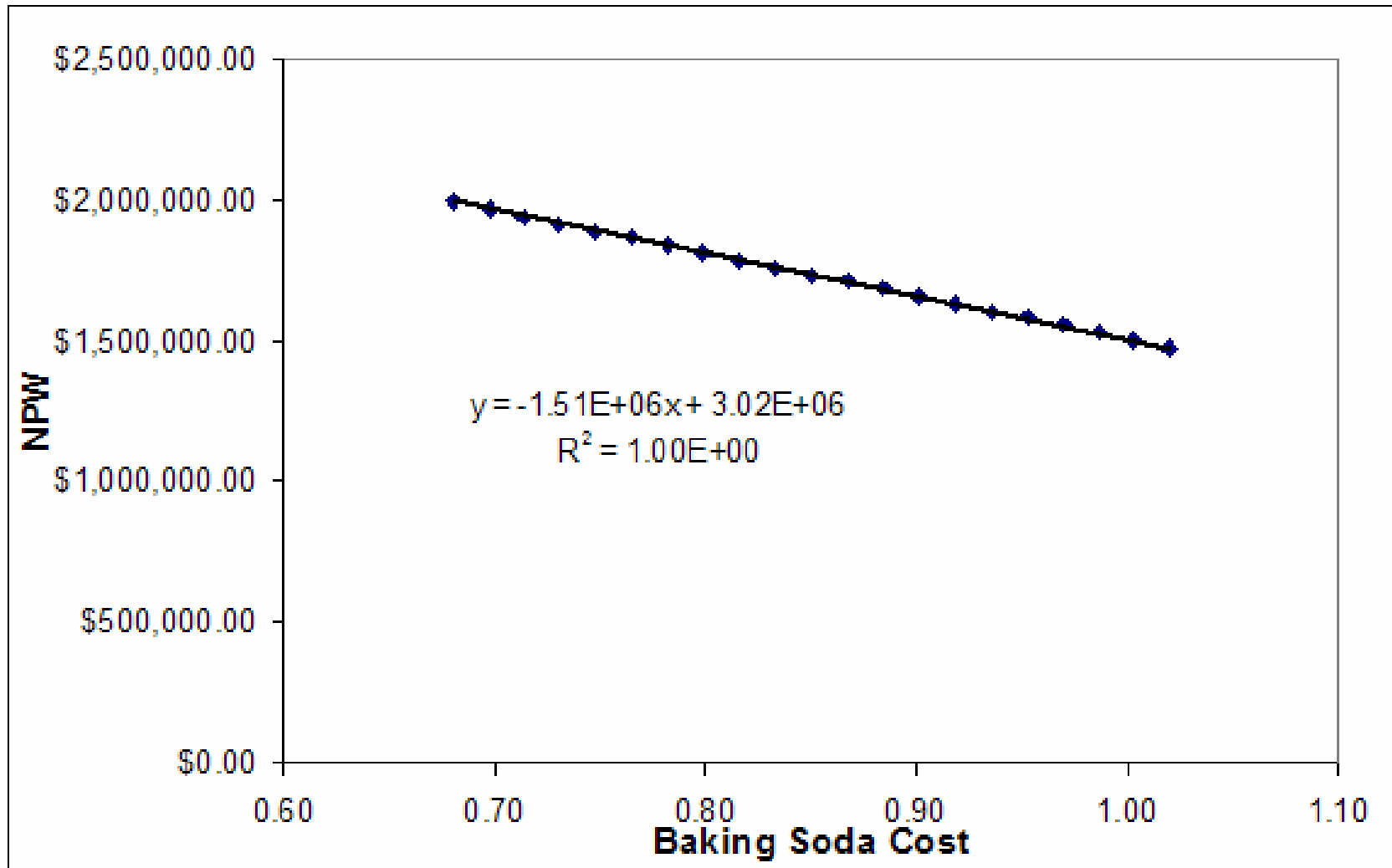
□ Strauss Plots

- Varied all raw materials 20% of 2007 selling price

□ Monte Carlo Simulations

- Varied all raw materials 20% of 2007 selling price

Strauss Plots





Cost

Strauss Plot Slope

Linalool

-150

PLGA

-400

Boric Acid

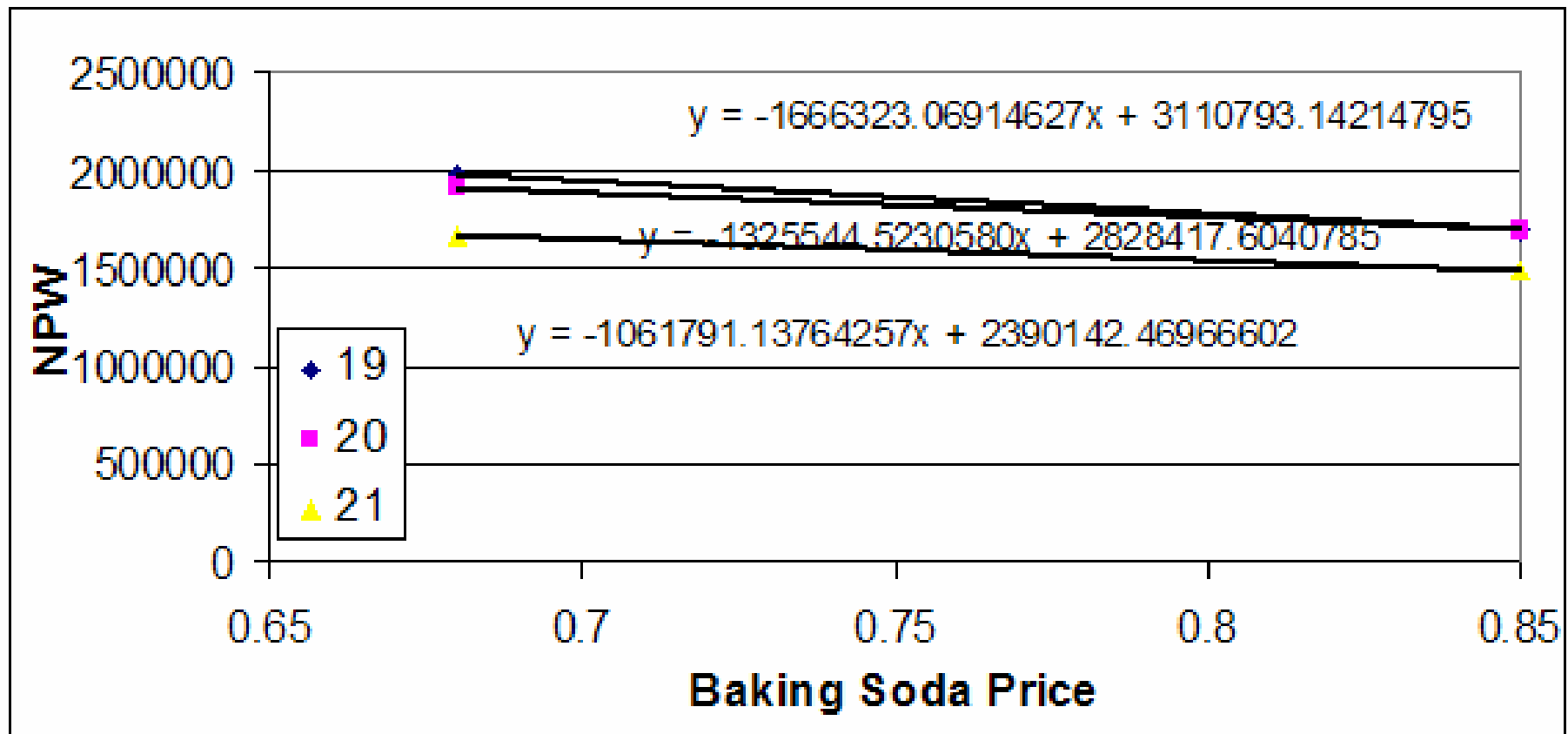
-3e5

Baking Soda

-1e6

Strauss Plots

- Sensitivity to Price



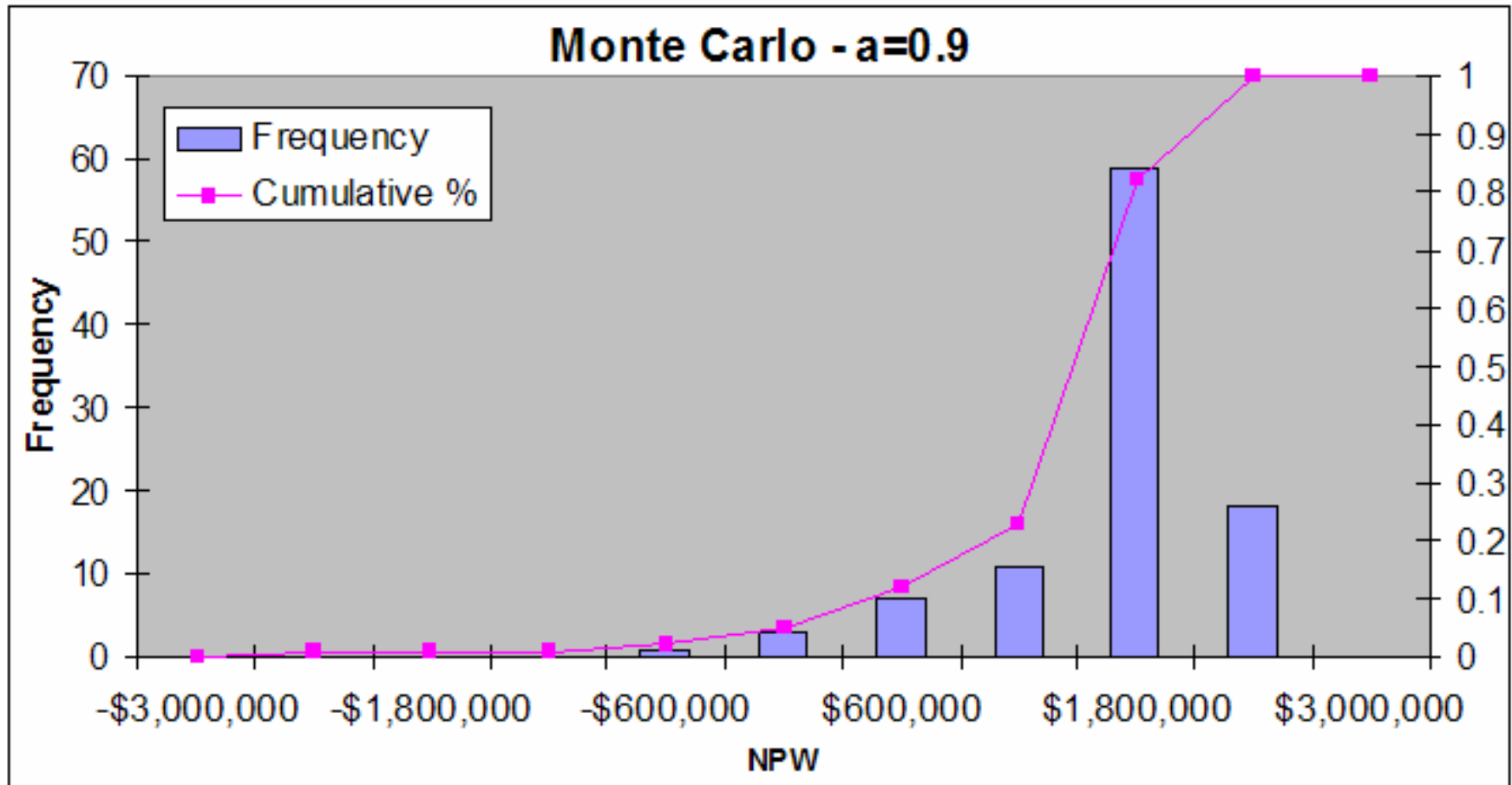
- Lower the price, higher the demand, and higher sensitivities

Strauss Plot Slopes

Price per container	Linalool	PLGA	Boric Acid	Baking Soda
\$19	-440	-162	-3.6e5	-1.6e6
\$20	-350	-129	-2.9e5	-1.3e6
\$21	-280	-123	-1.3e5	-1.0e6

As price goes down, demand goes up the NPW is a stronger function of the raw materials

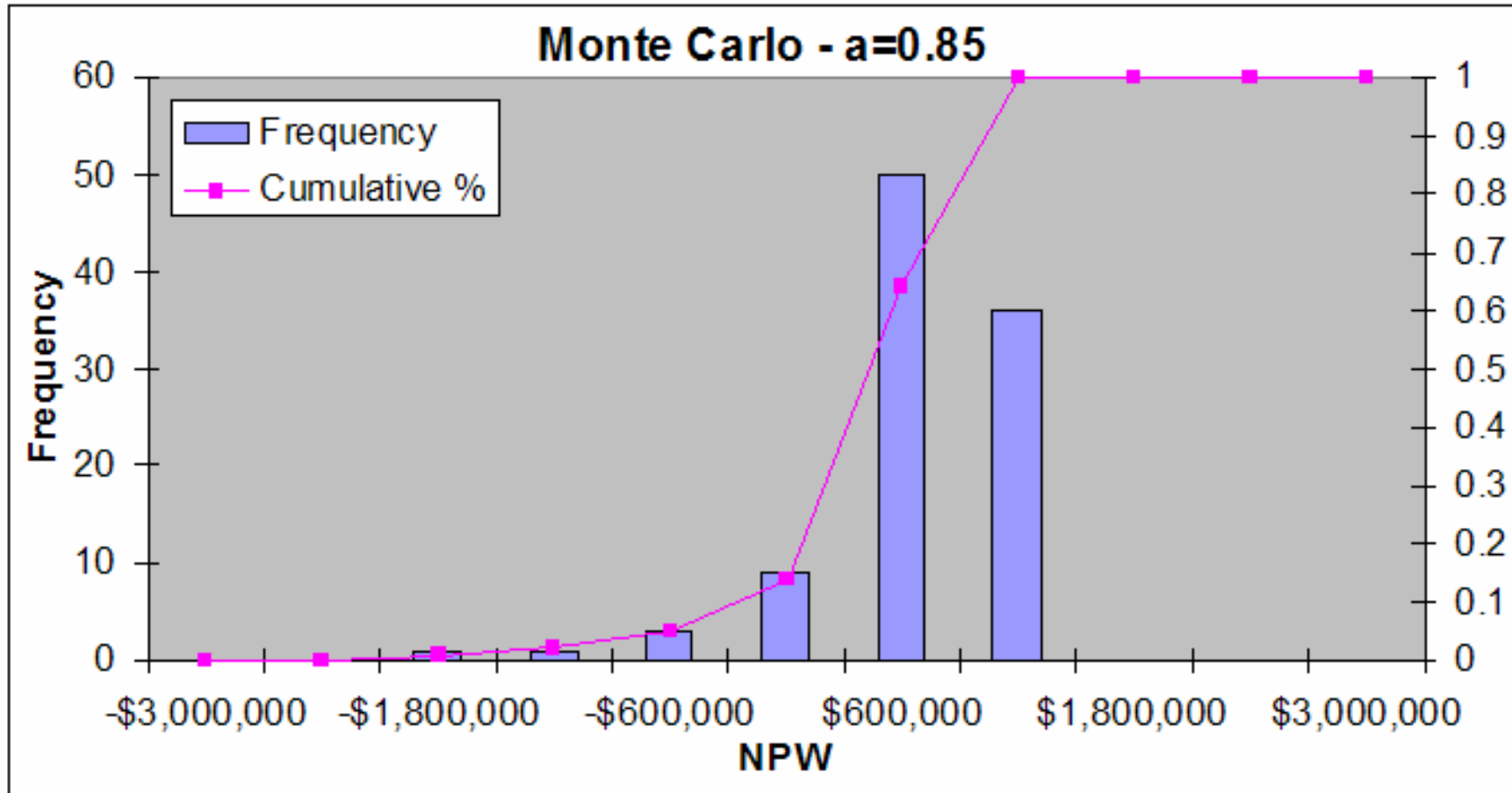
Monte Carlo Simulations – Y=54mill



5% of losing money

95% of making money

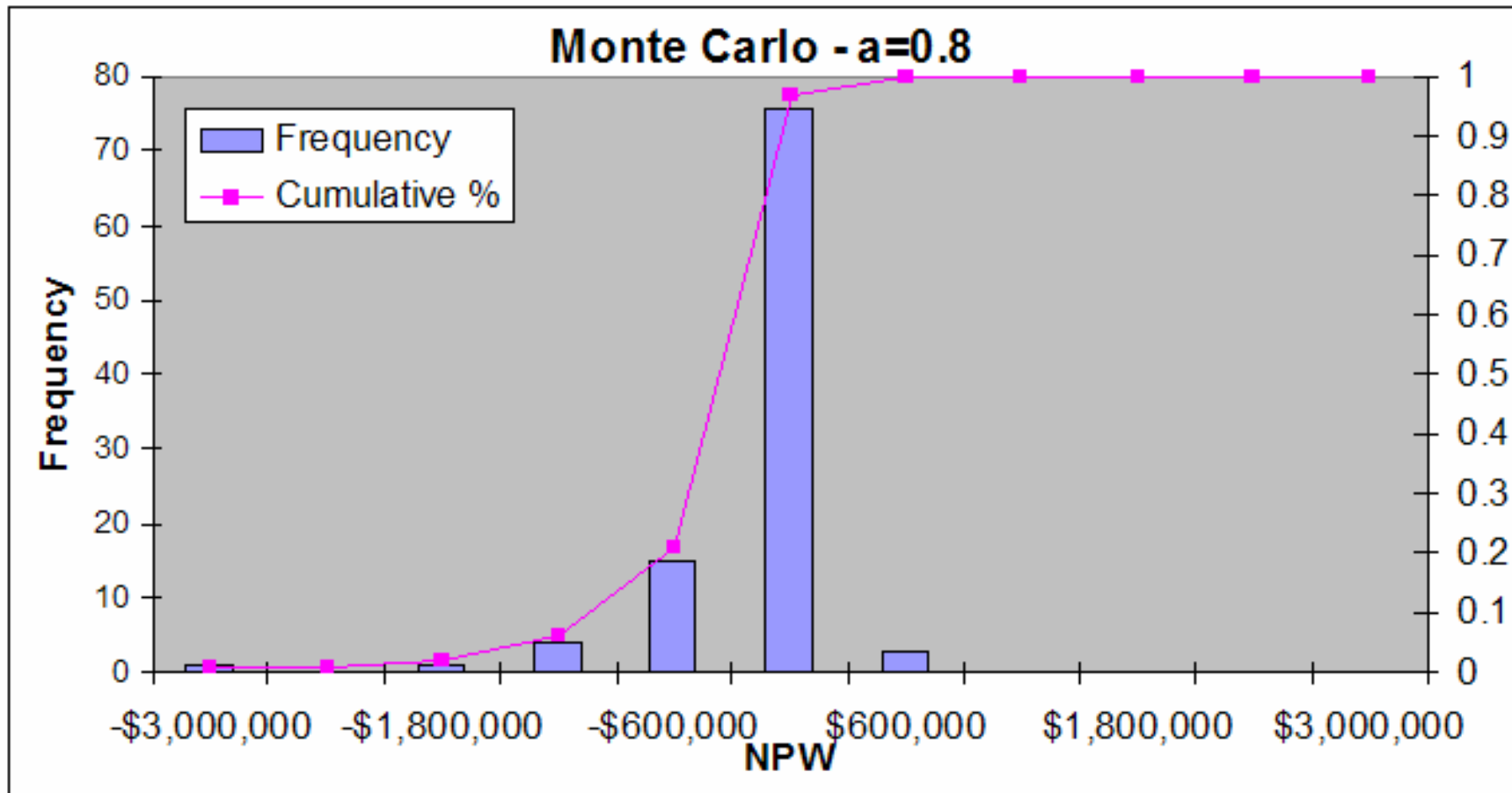
Monte Carlo Simulations – Y=54mill



14% of losing money

86% of making money

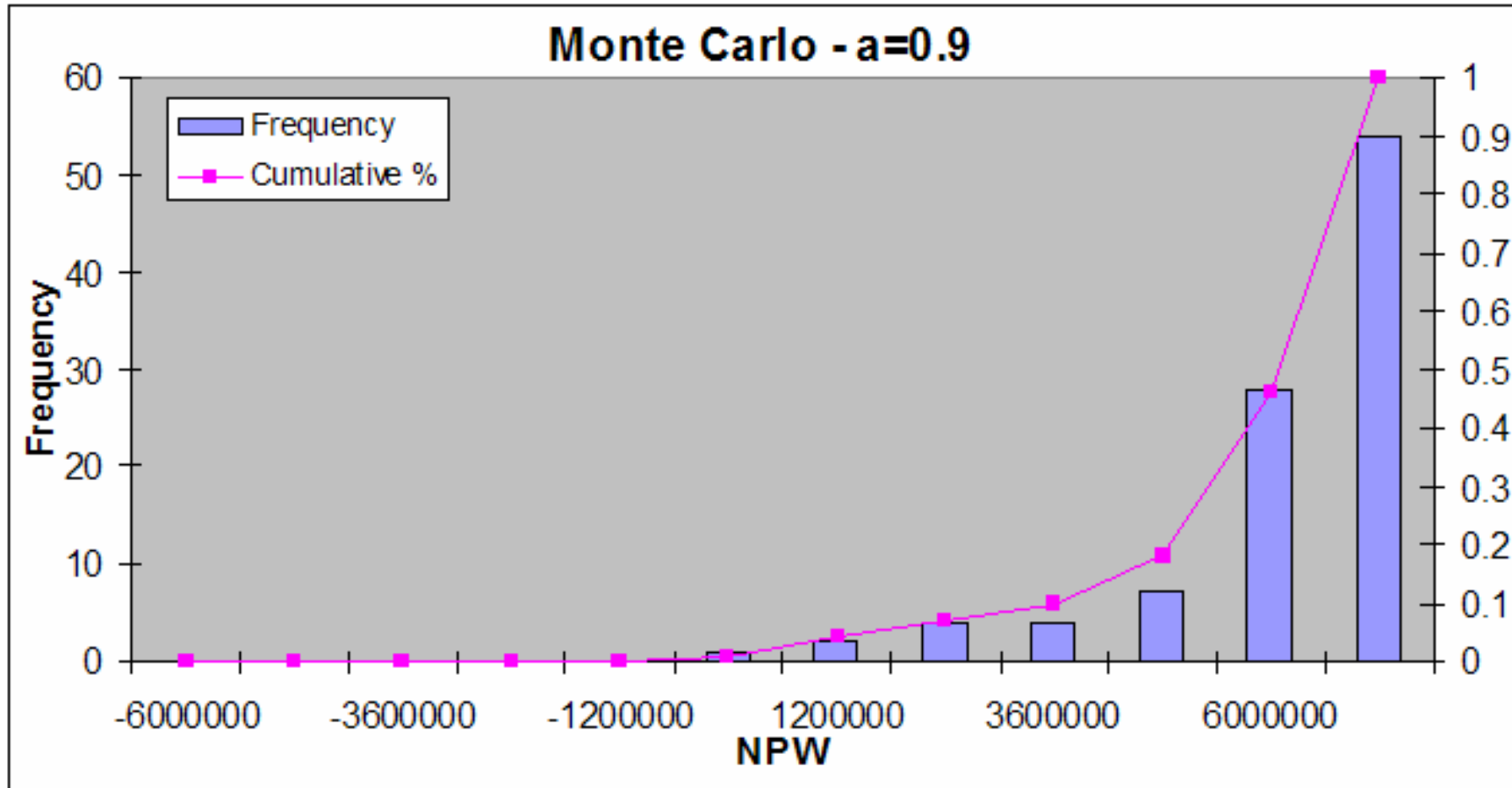
Monte Carlo Simulations – Y=54mill



97% of losing money

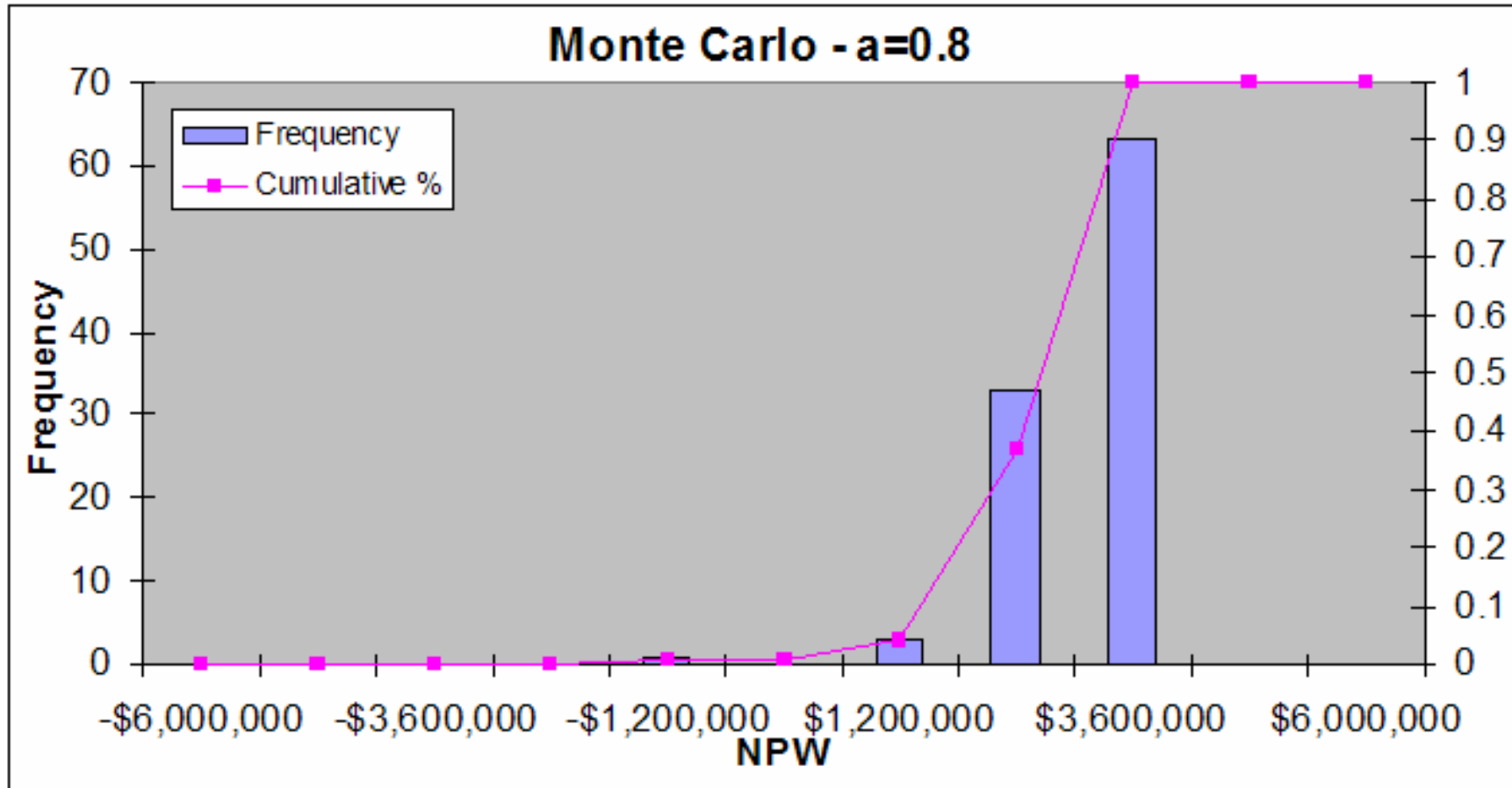
3% of making money

Monte Carlo Simulations – Y=97mill



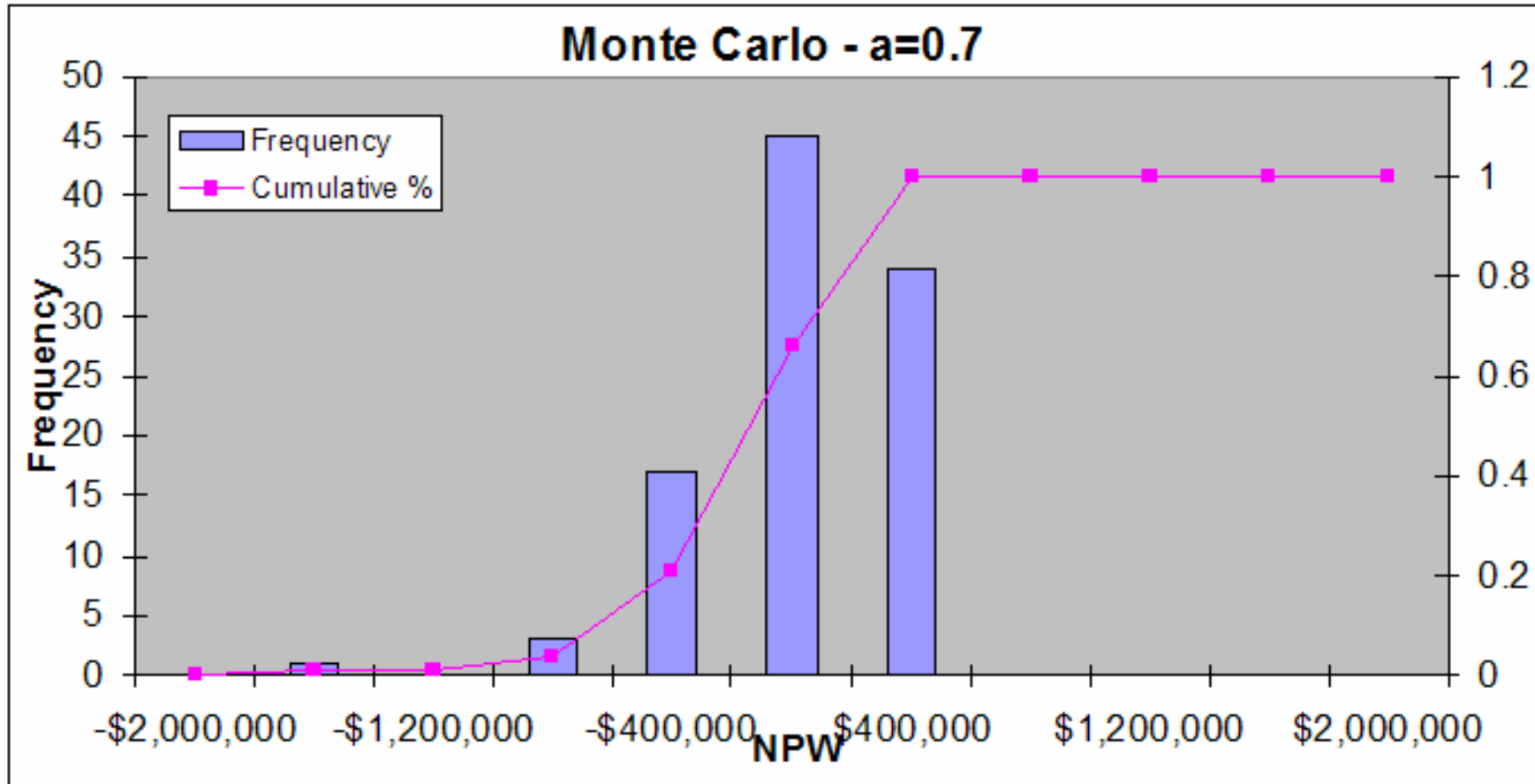
1% of losing money
99% of making money

Monte Carlo Simulations – Y=97mill



1% of losing money
99% of making money

Monte Carlo Simulations – Y=97mill



66% of losing money
34% of making money



Questions

Utility Questions

Utility	Wt.	U_{ours}	U_{theirs}	$U_{\text{theirs should be}}$
Duration - Linalool	0.19	13.90	9.50	0
Toxicity	0.09	7.50	7.50	7.5
PLGA-Scent Strength	0.22	16.40	11.00	0
Boric Acid	0.21	18.00	19.95	19.95
Baking Soda	0.15	14.90	7.30	7.3
What Scent	0.14	13.00	7.00	7
		83.70	62.25	41.75
		$\beta =$	0.73	0.50
		NPW	\$1,730,000	\$12,000,000

This table breaks down our conservative approach for the utility. When polled consumers stated for our product their would be a 0 utility for a product that had no duration and no scent, yet we felt that to be conservative we should give our competitor 50% of the utility so that we would not be making unrealistic amounts of money. This table shows how much we make with the conservative approach and how much we would have made if the competitor would have had a 0 utility for both. Another implication of our model being conservative with the utility for the fragrance of the competitor is that it gave us the freedom to look into the fragrance market also, which is very important. It would be like comparing apples and oranges if we would have excluded that.

Equipment Costs

Equipment Costs		
Unit	Capacity (lbs)	Cost(2007)
solids storage	850	\$780.00
sonicator	1.62	\$5,000.00
roto vap	1.62	\$3,200.00
centrifuge	1.62	\$1,400.00
freeze dryer	1.62	\$1,800.00
mixer	850	\$20,152.00
Total Equ't Cost		\$32,000.00

TCI, FCI, Working Capital

Capital Investment		
Direct Costs	% of Purchased Equ't	
Purchased Equipment Delivered	1	\$32,000.00
Purchased-equipment installation	0.47	\$15,040.00
Instrumentation and Controls	0.36	\$11,520.00
Piping	0.68	\$21,760.00
Electrical Systems	0.11	\$3,520.00
Rent		\$60,000.00
Buildings	0.18	\$5,760.00
Yard Improvements	0.1	\$3,200.00
Service facilities	0.7	\$22,400.00
Total Direct Plant Cost		\$175,200.00
Indirect Costs		
Engineering and Supervision (2 Eng 70K)		\$140,000.00
Construction Expenses	0.41	\$13,120.00
Legal expenses	0.04	\$1,280.00
Contractor's fee	0.22	\$7,040.00
Contingency	0.44	\$14,080.00
Total Indirect Plant Cost		\$175,520.00
Fixed Capital Investment		\$350,720.00
Working Capital		\$175,360.00
Total Capital Investment		\$526,080.00

ROI and PBP questions

Yr	Sales	Costs	Annual Cash Flow	d	r	$[(e-r)/r]e^{-rj}$	Present Worth
1	\$7,300,396.28	\$6,809,171.87	\$320,076.67	\$780.80	\$0.00	0.93	\$299,439.14
2	\$7,519,408.17	\$7,013,423.60	\$329,670.77	\$780.80	\$0.00	0.81	\$268,157.45
3	\$7,744,990.42	\$7,223,802.89	\$339,552.69	\$780.80	\$0.00	0.71	\$240,144.35
4	\$7,977,340.13	\$7,440,493.55	\$349,731.08	\$780.80	\$0.00	0.61	\$215,058.22
5	\$8,216,660.33	\$7,663,684.93	\$360,214.81	\$780.80	\$0.00	0.53	\$192,593.16
6	\$8,463,160.14	\$7,893,572.05	\$371,013.06	\$780.80	\$0.00	0.46	\$172,475.25
7	\$8,717,054.95	\$8,130,355.79	\$382,135.25	\$780.80	\$0.00	0.40	\$154,459.20
8	\$8,978,566.59	\$8,374,243.04	\$393,591.11	\$780.80	\$0.00	0.35	\$138,325.36
9	\$9,247,923.59	\$8,625,446.91	\$405,390.64	\$780.80	\$0.00	0.30	\$123,877.05
10	\$9,525,361.30	\$8,884,186.89	\$417,544.16	\$780.80	\$0.00	0.27	\$110,938.14
10end	\$0.00	\$0.00	\$0.00	\$0.00	\$24,192.00	0.24	\$5,806.08
						Sum	\$1,921,273.42
			NPW				
			\$1,735,801.42				
	16 oz cont	Revenue		TCI	FCI	ROI=Np,avg/TCI	PBP (yrs)
	375000	\$19.47		\$403,328.00	\$350,720.00	86.00%	1.01