All About Aerosols

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Purpose of this presentation

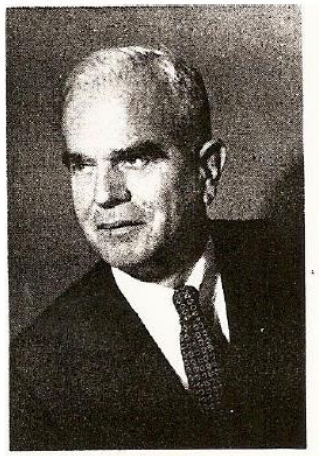
- Many formulating chemists are comfortable making liquids, creams, lotions, and gels, but when it comes to aerosols, there seems to be a general lack of know-how.

What is an aerosol?

- In the most broad sense, an aerosol consists of very fine particles of a liquid or solid suspended in a gas (i.e. air)
- Aerosol is a commonly-used term for a pressurized container which releases a spray or foam when actuated

A Very Brief History: The first example of a pressurized aerosol

History



- 1943 USA: Department Of Agriculture researchers Goodhue & Sullivan develop a small aerosol can pressurized by a liquefied gas. Service men spray malaria infested mosquitoes.

From there, things quickly escalated as the Personal Care industry discovered exciting new uses for the technology:

And speaking of Right Guard…

My involvement with aerosols

- My first job out of college was in the Product Development lab at Herbert V. Shuster, Inc., where I worked with Dr. Bernie Siegal, who was known to us as "the inventor of Ban Roll-on and Right Guard"
- My first, very limited aerosol exposure included:
  - Fragrancing "bulk" samples for private label, "Gillette Foamy"
  - Placing aerosol cans of antiperspirant on stability
  - Creating bulk for an aerosol silver polish, and then taking them to an aerosol filler in Webster MA to magically transform them into finished sprays
  - I did not have a firm grasp on the technology behind creating aerosols
- Imagine my surprise when overhearing that my private label client had been in the news a few years back…

Suddenly I developed a new mistrust of aerosol plants:

AROUND THE NATION; 25 Injured in Explosion At Aerosol Can Factory

AP

A fiery explosion flashed through an aerosol can factory today, searing skin from the faces and bodies of some workers and blowing the clothes off others. At least 25 persons were injured.

Frank McGaughey, chairman of the Selectmen in the town of 10,000, said that

National news is on pages A16-18 and B6-11. 16 workers had been severely burned. Several victims were flown by helicopter to burn clinics in Boston, 15 miles to the north.

Witnesses said flames shot 50 feet into the air after the blast, which ripped most of the metal siding off the Aerosol Research Laboratory building, flattened its walls and tore a hole in the roof.

Regardless, in 2006 I decided to confront my fears and took a job with Pharmasol Corporation, a small manufacturer of aerosol products

- Quickly, I was learning about "propellant tank farms", aerosol filling lines, and gashouse safety
- I learned about cans, valves, actuators…a lot of things about aerosols that I simply took for granted
- I started working closely with aerosol formulas, and learned which technologies could cross over well from non-aerosol formulas, and which things could not. Like hand sanitizer gel…
- Perhaps most importantly, I learned not to fear working with **highly flammable propellant gases**, but instead how to handle them properly and safely

Why choose aerosol?

- Convenient
- Easy to use
- Controlled Application
- Compact and Portable
- Long-lasting
- Uniform Spray
- Protected/tamper proof

Basic Anatomy

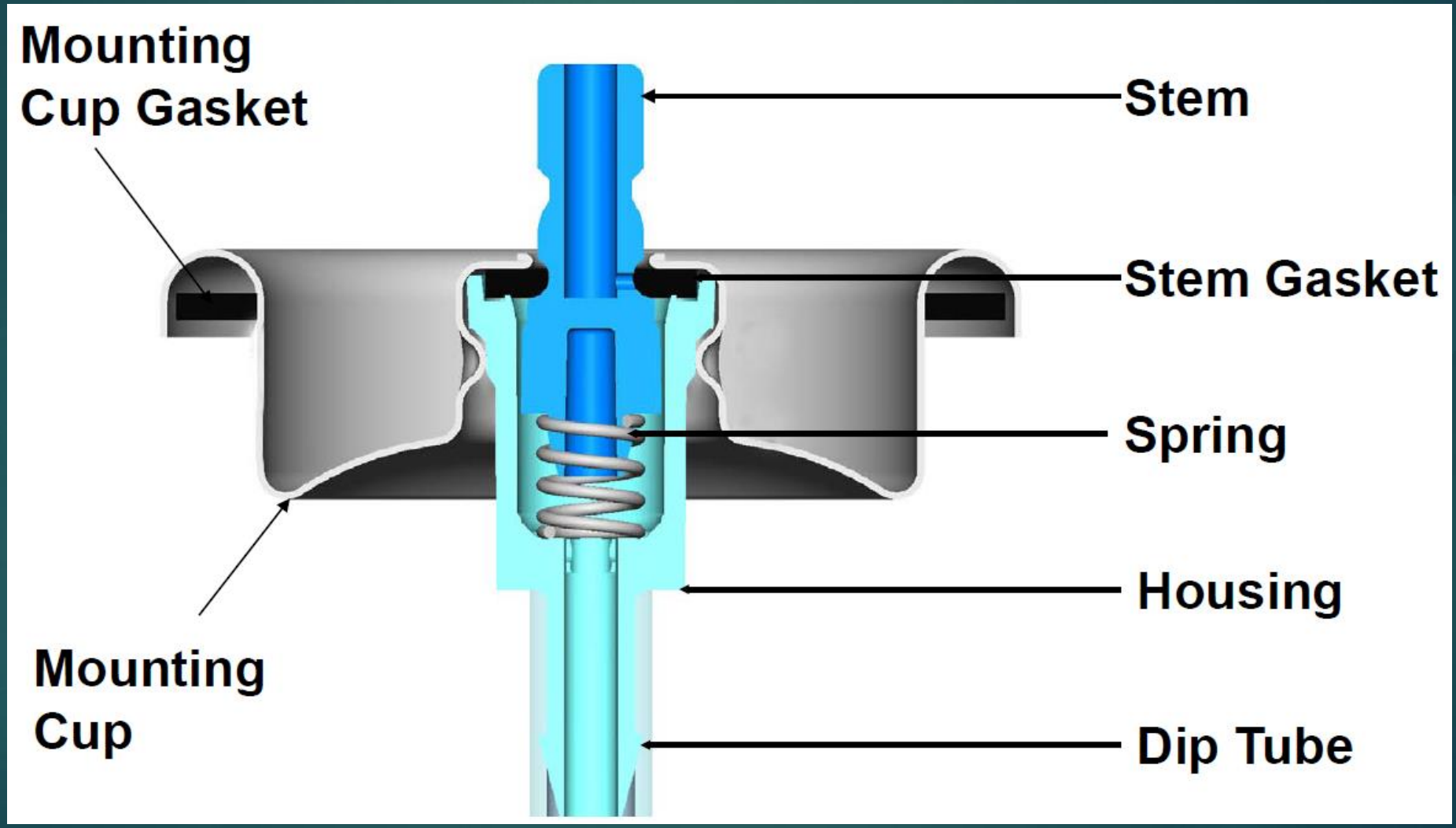
- Canister
  - Aluminum or Tinplate?
  - Pressure rating(buckle/burst)
    - 2P, 2Q, 18 bar, etc.
  - Lining choices
    - EP, PAM, Micoflex
  - Sizes and shapes

Basic Anatomy

Basic Anatomy

- Valve
  - 1” and 20mm
  - Upright – dip tube
  - Inverted
  - 360
  - Continuous vs/ metered
  - Stem orifice impact

Basic Anatomy



Basic Anatomy

- Actuator
  - Orifice size
  - Button type
  - Specialty
  - Foamers

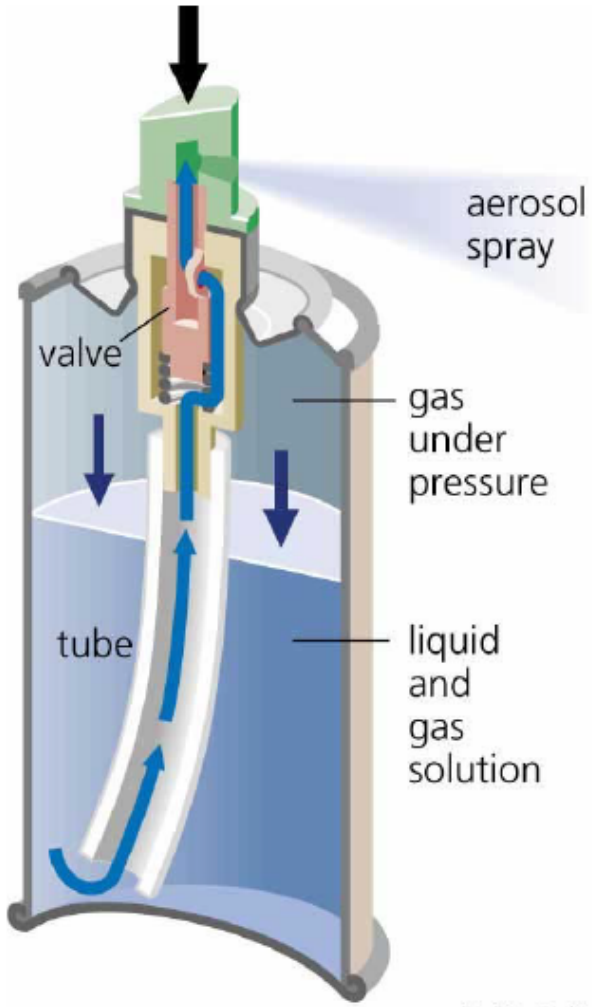
Basic Anatomy - Sprays

Basic Anatomy - Foams

How do I know which valve and actuator to use?

- This is where your valve supplier is your best resource
  - Send them the bulk product, and tell them what type of product you are making
  - List any specific spray or foam properties that you are after, i.e. light spray, dries quickly, ideal spray pattern, etc.
  - Tell them the type of propellant you are going to use, and the concentrate/propellant ratio
  - The valve supplier will then take your product into their lab and will test it with a variety of valves and actuators, to find combinations which meet your requirements

Operation



Pressure on the actuator moves the stem down.

This breaks the seal between the gasket and the stem.

The stem is exposed to the product/propellant in the container. (i.e. the valve is open)

Pressure inside the container pushes the product through the valve to the outside of the container.

By releasing the actuator, the spring returns the stem orifice to the sealed position (i.e. the valve is closed)

Propellants

- Chlorofluorocarbons – BANNED, ozone-depleting
- Hydrocarbons – Naming convention related to vapor pressure in psi
  - n-Butane A17
  - Isobutane A31
  - Propane A108
  - Other blends – Custom blends can be prepared to obtain different can pressures, i.e. A46, AP70, A63.

Propellants

- Fluorocarbons
  - Fluorocarbon 152a
  - 134a
  - 1234ze “Solstice”
- DME – Dimethyl Ether - Water solubility
- Custom Blends - Hydrocarbon propellants can also be blended with other propellants, like 152a and DME, to reduce VOC content, increase water-solubility, etc.

Propellants

- Other Options
  - BOV
  - Bag-in-can
  - etc.
- Pressurized gas, air, nitrogen, etc.

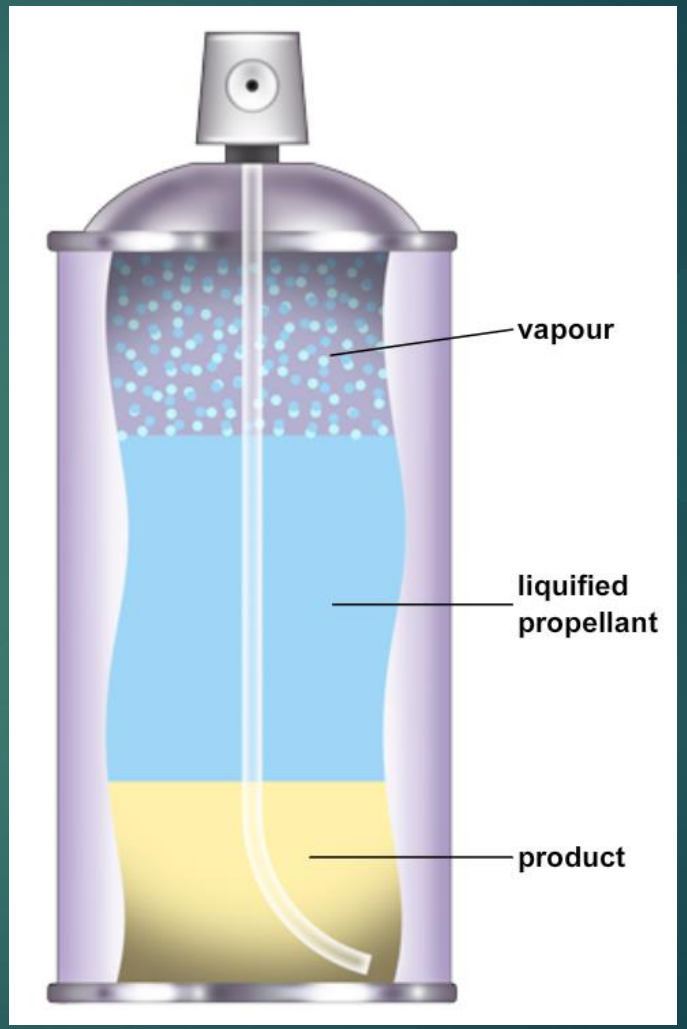
- Film pouch (Aptar, Coster, Lindal, Summit)
- PET (Power Container)

Propellants

- VOC considerations
  - CARB, restrictions for % VOC in different aerosol categories
  - VOC-exempt propellants
    - 152a
    - 134a – non-flammable
    - 1234ze- also non-flammable
- Other considerations, i.e. Europe

Types of Aerosols

- Single-phase vs. dual-phase
- Sprays
- Foams



Formulating

- Aerosol formulas are expressed in two ways:
  - As "Bulk" or "Concentrate" – This is the portion of the formula without the inclusion of the propellant, expressed as 100% w/w. This is typically the formula as it will be batched, and added to the can.
  - As "Finished Product" – This is the entire can contents, concentrate AND propellant, expressed as 100% w/w.

Example Formula 1: Shaving Cream

Chemical Name	Trade Name	% w/w bulk	%w/w/ finished
Water	Water	**85.67**	82.24
Stearic Acid, triple-pressed	Stearic Acid	**6.55**	6.29
Laureth-23	Brij 35	**2.17**	2.08
Triethanolamine	TEA99	**3.38**	3.24
Sodium Laureth Sulfate (30%)	SLES	**0.82**	0.78
Fragrance (proprietary)	Fragrance	**0.40**	0.39
BHT	BHT	**0.02**	0.02
Extract Blend		**0.50**	0.48
Tilia Cordata Flower Extract	Linden Extract		
Aloe Barbadensis Leaf Extract	Aloe Vera		
Cucumis Sativus (Cucumber) Fruit Extract	Cucumber Extract		
Propylene Glycol	Propylene Glycol		
Cetraria Islandica Extract	Iceland Moss Extract		
Liquid Germall Plus	Liquid Germall Plus	**0.50**	0.48
Propellant	A46	~	4.00
	TOTAL	**100**	100
96% bulk, 4% A-46			

Example Formula 2: Hairspray

Ingredient	Trade Name	%w/w finished	VOC	%w/w bulk
SDA 40B 200pf	SDA 40B 200pf	44.08	44.08	**67.82**
Polyurethane-14 (and) AMP-Acrylates	DynamX (28%)	15.00	3.75	**23.08**
Water		5.00		**7.69**
Triethyl citrate	Citroflex 2	0.15		**0.23**
Cyclopentasiloxane	DC 345	0.10		**0.15**
Ethylhexyl Methoxycinnamate	Octinoxate	0.10		**0.15**
Dimethicone Copolyol	Silsense DW-18	0.05		**0.08**
Fragrance	Honeysuckle	0.40		**0.62**
Actiphyte of honey	Actiphyte of honey	0.10		**0.15**
Panthenol	Panthenol	0.01		**0.02**
Vitamin E	Vitamin E	0.01		**0.02**
Propellant	152a	35		~
		100.00	47.83	**100.00**

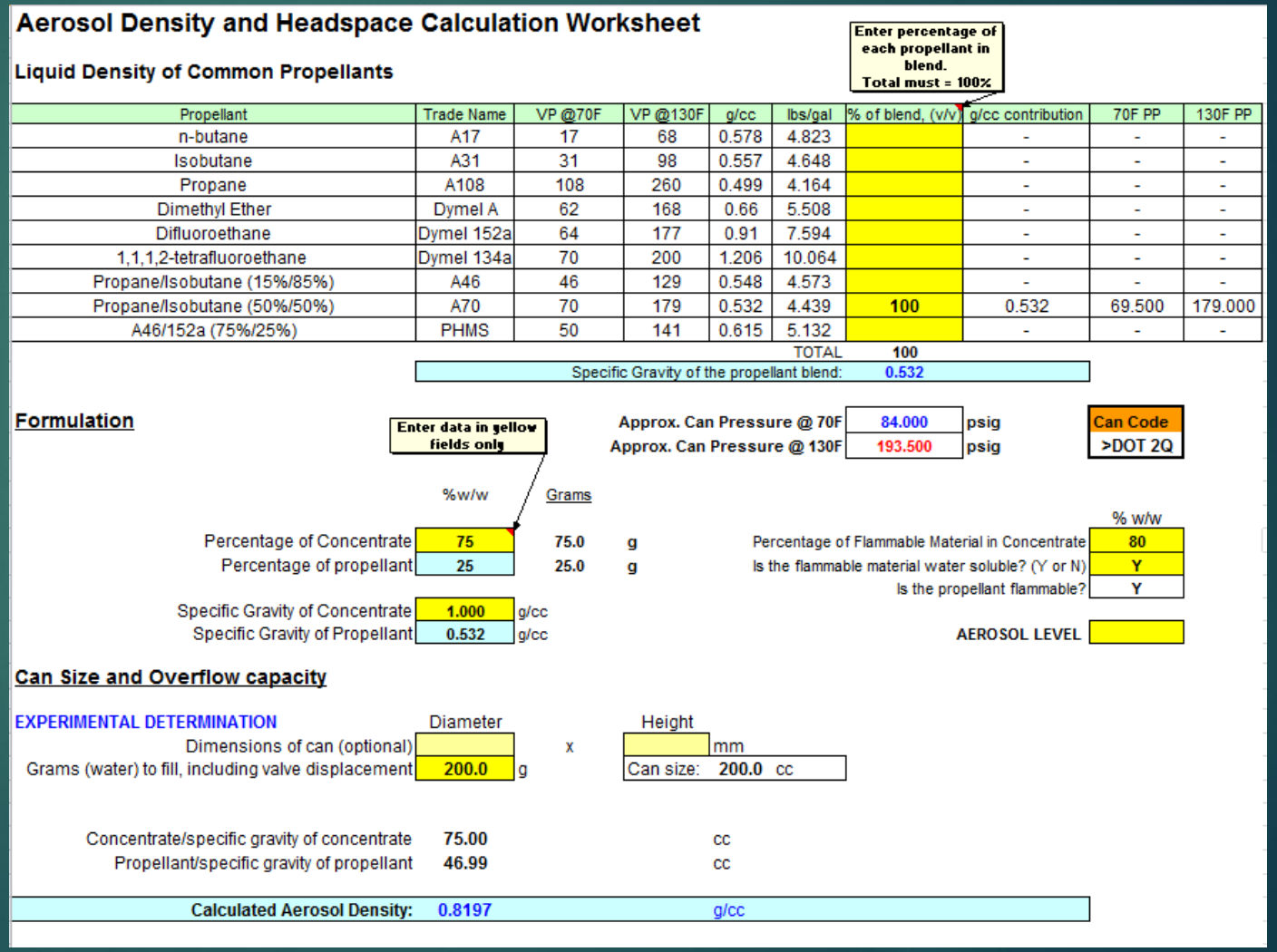
Propellant	152a		35	
Concentrate	Concentrate		65	

Filling Canisters

- Determine amount of concentrate and propellant to be filled
  - Concentrate is filled first
  - Valve is crimped onto canister
  - Propellant is added
- Lab filling – Concentrate added, manual crimping, pressure burette to add propellant
- Production filling – Piston fill concentrate, automated crimping, propellant injected through the valve stem by piston filler

Filling the can

- How much will fit into the can?
- Fill ratio
- Calculating how to fill, aerosol density



Aerosol Density and Headspace Calculation Worksheet

Liquid Density of Common Propellants

Enter percentage of each propellant in blend. Total must = 100%

Propellant	Trade Name	VP @70F	VP @130F	g/cc	lbs/gal	% of blend, (v/v)	g/cc contribution	70F PP	130F PP
n-butane	A17	17	68	0.578	4.823		-	-	-
Isobutane	A31	31	98	0.557	4.648		-	-	-
Propane	A108	108	260	0.499	4.164		-	-	-
Dimethyl Ether	Dymel A	62	168	0.66	5.508		-	-	-
Difluoroethane	Dymel 152a	64	177	0.91	7.594		-	-	-
1,1,1,2-tetrafluoroethane	Dymel 134a	70	200	1.206	10.064		-	-	-
Propane/Isobutane (15%/85%)	A46	46	129	0.548	4.573		-	-	-
Propane/Isobutane (50%/50%)	A70	70	179	0.532	4.439	100	0.532	69.500	179.000
A46/152a (75%/25%)	PHMS	50	141	0.615	5.132		-	-	-
					TOTAL	100			

Specific Gravity of the propellant blend: 0.532

Formulation

Enter data in yellow fields only

Approx. Can Pressure @ 70F: 84.000 psig
Approx. Can Pressure @ 130F: 193.500 psig

Can Code: >DOT 2Q

	%w/w	Grams			% w/w
Percentage of Concentrate	75	75.0	g	Percentage of Flammable Material in Concentrate	80
Percentage of propellant	25	25.0	g	Is the flammable material water soluble? (Y or N)	Y
				Is the propellant flammable?	Y
Specific Gravity of Concentrate	1.000	g/cc			
Specific Gravity of Propellant	0.532	g/cc		AEROSOL LEVEL	

Can Size and Overflow capacity

EXPERIMENTAL DETERMINATION	Diameter		Height	
Dimensions of can (optional)		x		mm
Grams (water) to fill, including valve displacement	200.0 g		Can size: 200.0 cc	

Concentrate/specific gravity of concentrate	75.00	cc
Propellant/specific gravity of propellant	46.99	cc
Calculated Aerosol Density:	0.8197	g/cc

Filling in the Lab vs/ Filling in Production

- Can size, and conc/prop fills

Headspace Calculation

7.5% is safe for all containers
4.5% is safe for containers w/ concave base, or glass containers (checked after filling)

Can Size and Overflow Capacity	200.0	cc	
Percentage full	80	%	(use 80% as default)
Aerosol Density/Total Fill Weight	131.2	g	or 160 cc
	4.6	ounces (dry weight)	
	4.4	fluid ounces	

This represents the maximum fill allowable for this can, not the label claim

Sample Filling Amounts

Can size 200.0 cc

Total Volume fill	160	cc	
Concentrate	98.4	cc, or	98.4 grams
Total Propellant	61.6	cc	

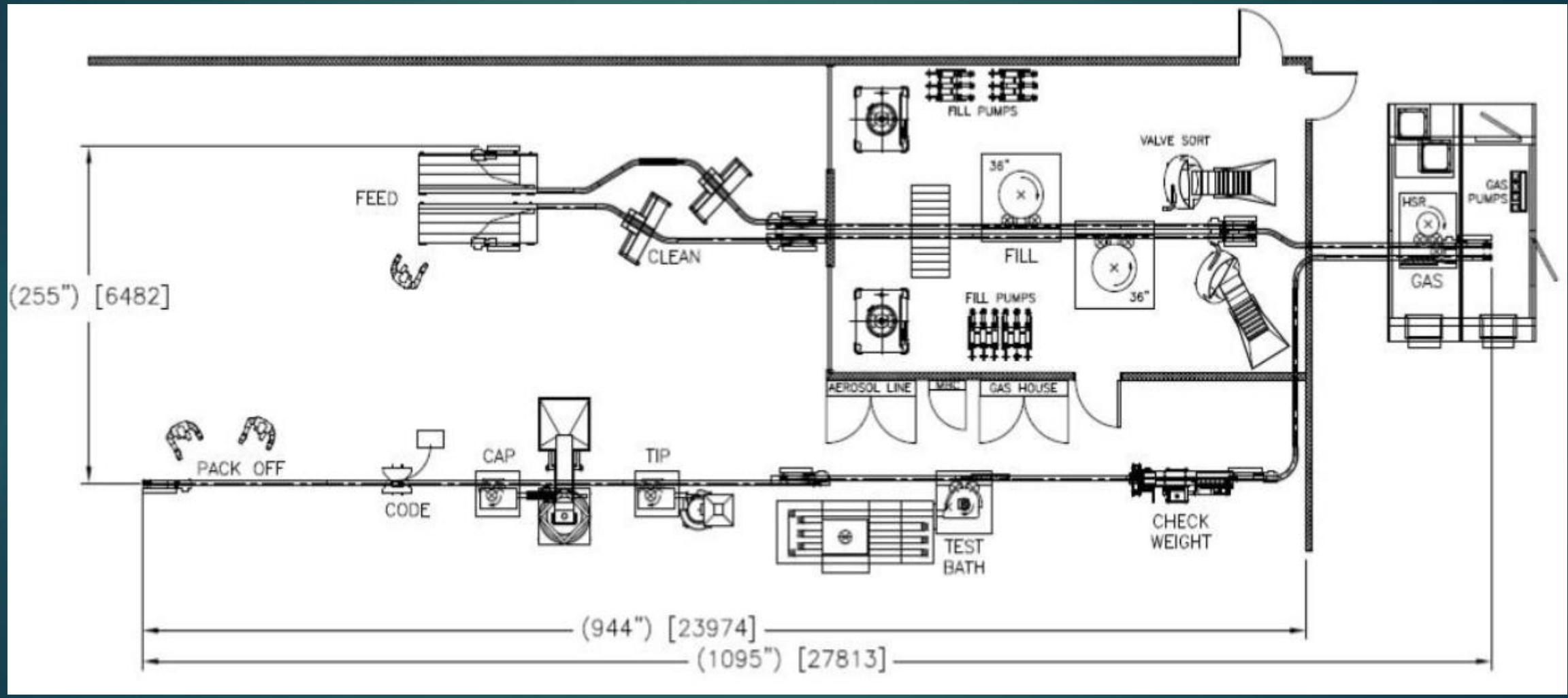
Amounts of individual propellants to be added		
A17	-	cc
A31	-	cc
A108	-	cc
DME	-	cc
Dymel 152a	-	cc
Dymel 134a	-	cc
A46	-	cc
A70	61.6	cc
PHMS	-	cc
TOTAL	61.6	

Lab Filling Equipment

Manual Internal 1” Crimp

Manual Burette TTV Gasser

Production Filling Line



Testing

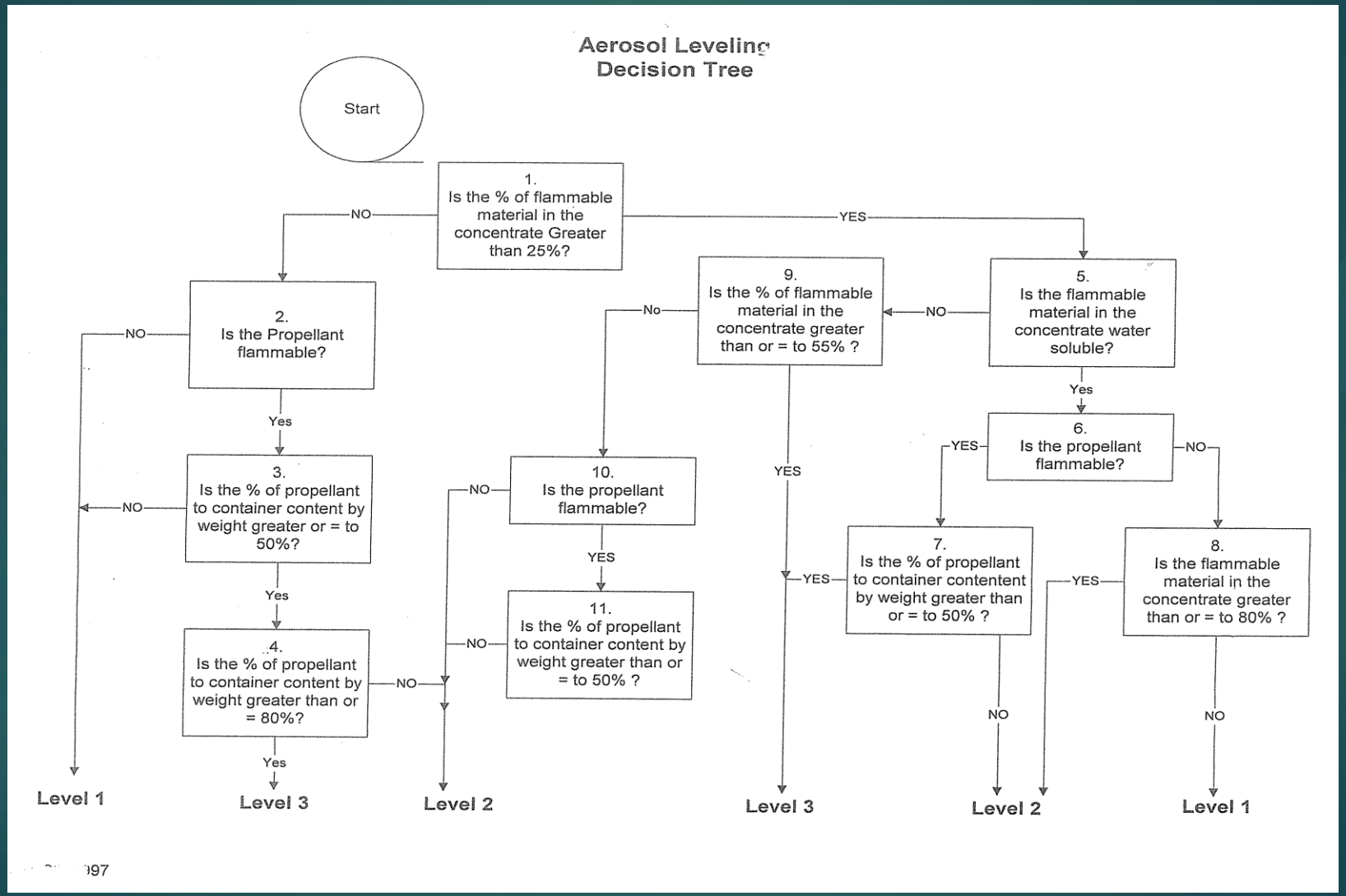
- Pressure
- Compatibility/Corrosion/Stability
- Gasket Swell
- Spray Rate/ Spray Pattern
- Foam quality, foam density
- Rx: Time to break, birefringence
- Extrusion – Label Claim in grams
- Flammability: Flame Extension/Flashback
- Respirable Particles

Safety

- Flammability, explosion risks
- Shipping Considerations
- Storage and Handling

  DOT Class 1, 2, 3 aerosols

Aerosol Level - DOT



This concludes our very quick overview of aerosol technology

Questions?

Other resources:

- "Aerosol Technology" short course, given by the Center for Professional Advancement (CfPA) in New Brunswick, NJ

- Spray Technology & Marketing Magazine

And finally…

- If you are looking for assistance with developing or commercializing an aerosol product, give us a call and we will be happy to discuss it with you.
- Pharmasol is a full service contract manufacturer located nearby, in S. Easton, MA.
- We specialize in aerosol (and liquid) filling of Rx, OTC and cosmetic products.

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PHARMASOL

Thank you!

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