Effect of Organo-Functional Additives on Silicone Elastomers: Providing Useful & Desirable Properties for Cosmetic and Personal Care Products

By Fenbao (David) Zhang PhD*, Tony O'Lenick**, Rick Vrckovnik***

Abstract

Organo-silicone polymers are a very diverse class of compounds that find application in many types of formulations. The reason they have become so popular in cosmetic and personal care formulations is the fact that they can provide unique aesthetics in many skin formulations. Specifically, the presence of organo-silicone, in a properly chosen polymer can [1]; (1) lower Surface Tension, (2) provide a unique aesthetic, (3) form films (4)minimize pigment transfer and (5) foam hydroalcoholic solutions.

This article deals with the ability of organo-silicones to alter the aesthetics in skin care formulations of a class of silicone polymers generally known as **silicone elastomers, that have** an INCI designation of dimethicone / vinyl dimethicone crosspolymer.

Silicone Elastomers

The first question that arises in dealing with this class of compounds is "What exactly is a silicone elastomer?" Over the years there have been many definitions offered in the patent literature. As such, this practice has caused much confusion.

There are three different types of silicones [2]: (1) Fluids, (2) Elastomers and (3) Resins.

Silicone Fluids are linear compounds which means they lack crosslinking. As such, they are liquid. Even at high viscosity, the lack of crosslinking results in the ability to behave as a fluid and exhibit noticible flow behavior. Extremely viscous polymers in this class are referred to as silicone gums.

Silicone Elastomers - Elastomers have crosslinking introduced into the polymer. Crosslinking limits limits the ability of the polymer to freely rotate forming a more rigid network. Because of their limited concentration of crosslinked groups, elastomer polymers tend to self-heal.

As the crosslink density continues to increase, a rigid system, called a Silicone Resin is formed. As crosslinking increases, the ability of the polymer to rotate freely decreases significantly which results in the buildup of up a more rigid network.

The difference between a silicone elastomer and a silicone resin is shown in Figure 1. A resin will crumble when stressed, while an elastomer will self-heal.

Figure 1 [3]

Dimethicone/ Vinyl Dimethicone Crosspolymers

This type of silicone elastomer is made by the hydrosilylation reaction of a silanic hydrogen polymer (Si-H) and a terminal divinyl polymer. The reaction results in forming a new polymer reducing the Si-H and vinyl content to low levels. The INCI name therefore is misleading in that it implies there is vinyl silicone present in the final polymer. This is simply incorrect.

It can be said that the presence of the -CH2-CH2- group in the polymer, which comes from the vinyl group makes the elastomer an organo-functional polymer. The authors prefer to keep the organo-functional designation for polymers that contain higher concentrations of larger organic groups, including alkyl groups, fluoro alkyl groups, polyoxylakylene groups and the like.

* Siltech Corporation, ** Siltech LLC, *** Siltech Corporation

The addition of organo-functional compounds to elastomers results is one of the most potent methods of modifying aesthetics of cosmetic formulations with silicone elastomers.

In order to demonstrate the ability to alter elastomer aesthetics by addition modifiers, a standard dimethicone / vinyl dimethicone was evaluated by itself and with a 1% polymer add of an aesthetic modifier. This particular study was conducted using D5 as the solvent. Figure 8 outlines the compounds evaluated.

Product	INCI
Polymer A	Cyclopentasiloxane and dimethicone/vinyl dimethicone crosspolymer
Polymer B	Cyclopentasiloxane and dimethicone/vinyl dimethicone crosspolymer and polydecene and cetyldimethicone/bis-vinyldimethicone crospolymer
Polymer C	Cyclopentasiloxane and dimethicone/vinyl dimethicone crosspolymer and perfluorononyl dimethicone (proposed)
Polymer D	Cyclopentasiloxane and dimethicone/vinyl dimethicone crosspolymer and trimethylsiloxysilicate

Figure 2

Tactile Evaluation

The tactile feel of a silicone polymer is determined by its structure. The dry feel on skin is achieved by proper engineering of the polymeric structure. Indeed, it is a relatively small number of products that will provide the highly prized feel on skin that is the hallmark of superior cosmetic and personal care products.

Elastomer Property Descriptions

Initial Feel - Dry Powdery feel
Cushion - Length of time to spread
Play Time - Length of time cushion lasts
Final Polymer feel - Dry, waxy, none,
Other Properties - Transfer Resistance / Pigment Coating

Cushion

Cushion refers to the amount of compound that persists between the finger and forearm while rubbing on the forearm skin during application. Cushion can be thought of as a combination of viscosity and resistance to flow Honey has a great cushion because one can feel a large amount of material between their finger and forearm, whereas water has little to no cushion because there is little distance between finger and forearm.

Playtime

Playtime refers to the length of time the cushion persists. If the cushion is felt for a long period of time, the playtime is long. If the cushion collapses rapidly, the playtime is said to be short.

Cushion/Playtime

In most compounds the cushion and playtime are directly related. Honey has both a high cushion and a high playtime. There are materials that have a good cushion but rapidly collapse to have a low playtime.

The inclusion of a low concentration of selected additives into the resin can alter the materials aesthetics. All polymers described below were made with exactly the same base polymer to which an additive is added.

Polymer A

Parent Polymer
INCI Name: Cyclopentasiloxane (and) Dimethicone/Vinyl Dimethicone Crosspolymer

When one applies the polymer to the skin, by first putting the material on the index figure and then rubbing it on the forearm, there is a distinct dry powdery initial feel, as the rubbing continues the cushion while present, is "short", as is the play time. Ultimately, the product has a dry feel.

		10%	50%	90%
Material	Water	NC	NC	NC
	Triglycerides	NC	NC	NC
Solvents	Ethanol	NC	NC	C
	Propylene Glycol	NC	NC	C
	Isopropyl Glycol	NC	NC	C
	Acetone	NC	NC	C
Fatty Esters	Isopropyl Myristate	C	C	C
	Octyl Palmitate	C	C	C
	Isononyl Isononoate	C	C	C
	C_{12-15} Alkyl Benzoate	C	C	C
	Trioctyldodecyl Citrate	C	C	C
Hydrocarbons	Mineral Oils	NC	NC	C
	Isododecane	C	C	C
Silicones	Cyclopentasiloxane	C	C	C
	Dimethicone, 50 cts	C	C	C
	Isopropyl Phenyl Dimethicone	C	C	C

NC: not compatible; C: compatible

Table 1: Compatibility of Polymer A

Other polymers have the same compatibility as a result of the low 1% of Silicone additives added to the base polymer.

Polymer B

Parent Polymer with alkyl organi-silicone additive
INCI Name: Cyclopentasiloxane (and) Dimethicone/Vinyl Dimethicone Crosspolymer (and) Polydecene and Cetyldimethicone/Bis-Vinyldimethicone Crosspolymer

When this polymer is applied to the skin by first putting the material on the index figure and then rubbing it on the forearm, there s a distinct dry powdery initial feel, as the rubbing continues the cushion is present increased over Polymer A. The polymer has a longer play time. Ultimately, the product has a waxy feel. This feel is attributed to the added alkyl organo-functional silicone in the composition.

Polymer C

Parent Polymer with Spreading Agent

Assigned INCI Name: Cyclopentasiloxane (and) Dimethicone/Vinyl Dimethicone Crosspolymer (and) Perfluorononyl Dimethicone

When this polymer is applied to the skin by first putting the material on the index figure and rubbing it on the forearm, there is a distinct dry powdery initial feel, as the rubbing continues the cushion is decreased over Polymer A. The polymer has a very short play time. Ultimately, the product has a slick feel. This feel is attributed to the added alkyl organo-functional silicone in the composition.

Polymer D

Parent Polymer with Q Resin

Assigned INCI Name: Cyclopentasiloxane (and) Dimethicone/Vinyl Dimethicone Crosspolymer (and) Trimethylsiloxysilicate

When this polymer is applied to the skin by first putting the material on the index figure and rubbing it on the forearm, there is a distinct dry powdery initial feel, as the rubbing continues the cushion is present is decreased over Polymer A. The polymer has a short play time. Ultimately, the product has a slick feel. This feel is attributed to the added alkyl organo-functional silicone in the composition.

Polymer	Viscosity* cps, at 25°C	Additive	Solvent
Polymer A	580,000	None	D5
Polymer B	318,000	Polydecene and Cetyldimethicone/Bis-vinyldimethicone Crosspolymer	D5
Polymer C	340,000	Perfluorononyl Dimethicone	D5
Polymer D	540,000	Trimethylsiloxysilicate	D5

* Viscosity was measured by a Brookfield Synchro-Lectric Viscometer, LV Spindle #4, and 0.6 rpm at 25 °C

Table 2:Viscosity of Polymers at 25 °C

The effect of the additive on viscosity is clear from the data in table 2, Polymer B and Polymer C are very much lower than the Polymer A and D. Additives will alter the viscosity as well as aesthetics.

Sensory Parameters	A	B	C	D
Before Absorption				
Wetness (1=dry, 10=wet)	3.10	3.00	3.40	3.30
Spreadability (1=difficult, 10=easy)	3.70	3.80	4.00	3.90
Tackiness (1=not tacky, 10=tacky)	3.00	3.10	2.90	3.00
Absorbency (1=slowly, 10=fast)	7.00	7.10	6.90	7.00

Table 3 Initial Feel (Qualitative Property; Quantitatively Described)

Formulations

In order to show the effect of added organo-silicone polymers to the elastomer, the following formulations were prepared.

1. O+Si/W Moisturizer Formulation of O+Si/W Moisturizer

1. A Formula of O+Si/W Moisturizer

Ingredients	FC345A w/ Polymer A Wt%	FC345B w/ Polymer B Wt%	FC345G w/ Polymer C Wt%	FC345H w/ Polymer D Wt%
Part A				
D.I. Water	83.80	83.80	83.80	83.80
Biosil BB SMC	4.00	4.00	4.00	4.00
Part B				
Dimethicone, 5 cst	6.00	6.00	6.00	6.00
Sepigel 305	2.00	2.00	2.00	2.00
Polymer A	**4.00**	**0**	**0**	**0**
Polymer B	**0**	**4.00**	**0**	**0**
Polymer C	**0**	**0**	**4.00**	**0**
Polymer D	**0**	**0**	**0**	**4.00**
Part C				
Liquid Germall Plus	0.20	0.20	0.20	0.20
Total	**100.00**	**100.00**	**100.00**	**100.00**

Procedure:

1. Combine Part A, mix well.
2. Combine Part B, blend well. Add Part B into Part A under mixing, until homogenized.
3. Add Part C, mix well.

1. B Analysis of O+Si/W Moisturizer

Specifications	FC345A w/ Polymer A	FC345B w/ Polymer B	FC345G w/ Polymer C	FC345H w/ Polymer D
Viscosity (cps)	37,000	37,400	37,600	37,000
Specific Gravity (g/mL)	0.9848	0.9847	0.9841	0.9869
pH	6.12	6.14	6.13	6.12
Appearance	White Cream	White Cream	White Cream	White Cream
Stability @ RT	Good	Good	Good	Good
Stability @45 C	Good	Good	Good	Good
Feel (1-10, 10 the best)	9.0	9.1	9.1	9.1
Compatibility	Good	Good	Good	Good

All creams showed good compatibility. Creams were very smooth, soft, silky powdery feel on skin. Polymer A had the most dry after rub in, Polymer B gave a slightly more waxy feel, and Polymer C gave more spreadbility on the skin.

2. Long-wear Foundation

2. A Formulation of Long-wear Foundation

Ingredients	FM624 A w/ Polymer A Wt%	FM624 B w/ Polymer B Wt%	FM624 G w/ Polymer C Wt%	FM624 H w/ Polymer D Wt%
Part A				
D.I. Water	40.80	40.80	40.80	40.80
Veegum Ultra	0.50	0.50	0.50	0.50
Propylene Glycol	6.00	6.00	6.00	6.00
Sodium Chloride	1.00	1.00	1.00	1.00
Part B				
Silube J1015-O-812	3.00	3.00	3.00	3.00
Cyclopentasiloxane	12.00	12.00	12.00	12.00
Siltech CE 2000	8.00	8.00	8.00	8.00
Silsurf 400R	10.00	10.00	10.00	10.00
Excel Mica JP-2	3.00	3.00	3.00	3.00
Hydrogenated lecithin	0.30	0.30	0.30	0.30
Polymer A	**10.00**	**0**	**0**	**0**
Polymer B	**0**	**10.00**	**0**	**0**
Polymer C	**0**	**0**	**10.00**	**0**
Polymer D	**0**	**0**	**0**	**10.00**
Unipure Yel. LC 182	0.74	0.74	0.74	0.74
Unipure Red LC 381	0.22	0.22	0.22	0.22
Unipure Black LC 989	0.07	0.07	0.07	0.07
Unipure LC 987 AS	3.68	3.68	3.68	3.68
Part C				
Bentone Gel VS-5 PC	5.00	5.00	5.00	5.00
Part D				
Giovarez AC-5099M	3.00	3.00	3.00	3.00
Part E				
Liquid Germall Plus	0.30	0.30	0.30	0.30
Total	**100.00**	**100.00**	**100.00**	**100.00**

Procedure:

1. Disperse veegum ultra in water until uniform, add the rest of Part A and mix well.
2. Combine Part B and blend well, check pigment dispersions.
3. Heat Part A and B to 75 °C respectively, add Part A into Part B with continuous agitation. Cool the batch to room temperature. So far it can be normal liquid foundation. If add Part C/D, it will be long-wear foundation.
4. Add Part C into Part A+B under mixing until homogeneous, then add Part D into batch until uniform.
5. Add preservative liquid germall plus under mixing for another 5 minutes.

2.B Analysis of Long-wear Foundation

Specifications	FM624 A w/ Polymer A	FM624 B w/ Polymer B	FM624 G w/ Polymer C	FM624 H w/ Polymer D
Viscosity (cps)	8,800	8,900	8,800	8,900
Specific Gravity (g/mL)	1.0601	1.0602	1.0610	1.0606
pH	6.48	6.49	6.51	6.50
Appearance	Beige liquid FD	Beige liquid FD	Beige liquid FD	Beige liquid FD
Stability @ RT	Good	Good	Good	Good
Stability @45 C	Good	Good	Good	Good
Feel (1-10, 10 the best)	9.0	9.0	9.1	9.1
Compatibility	Good	Good	Good	Good

Long-wear, silky, smooth, soft slippery powdery feel especially for the foundation FM624B/G/H

Conclusions

Elastomers, especially those modified by the simple addition of organo-functional silicone polymers are a powerful tool in altering the skin aesthetics in a very wide personal care products designed to be applied to the skin. This approach provides a choice of unique and varied skin aesthetic properties to cosmetic formulations. These aesthetics provide consumer perceivable differences in formulations in which the elastomer chosen is the only difference. This approach demonstrates that silicone elastomers with organo-functional components are useful aesthetic modifiers of skin care products.

References

1) *O'Lenick, Anthony, Silicones for Personal Care, Allured Publishing 2008, p.20*
2) *O'Lenick, Anthony Silicones for Personal Care, Allured Publishing 2008, p.42*
3) *O'Lenick, Anthony Silicones for Personal Care, Allured Publishing 2008, p.248*