Silicone: The Basis of a Perfect Formulation for Hair Care

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Abstract

The needs of today's consumers have led cosmetics formulators to look for new alternatives to help treat the hair after exposure to external agents such as the sun, combing, and drying as well as chemical products such as permanents and dyes. A major objective has been to develop formulations using ingredients that provide a repairing effect on the hair.

This paper describes the use of silicones as conditioning agents in shampoos, conditioners, and various anhydrous systems. It focuses on the use of silicone gum blends and organofunctional fluids as basic ingredients in hair care formulations and describes their physicochemical properties, benefits, and functional activity. Recommendations and guidelines for formulating with silicone conditioning agents and examples of prototype formulations for conditioning shampoos, conditioners, and anhydrous systems are also included.

Introduction

In response to consumer demands, cosmetic chemists are working to develop hair care products that will impart repairing and conditioning effects on the hair. Silicones can help meet these objectives.

Silicones are a family of polymers whose origins lie in the mineral quartz, or silica, which has the chemical formula SiO_2. Through reactions such as hydrolysis and condensation, the basic Si-O-Si-O chain or "backbone" structure of silicone is formed. The addition of different functional groups results in a variety of silicones with differing properties. The proper selection of an individual silicone for an application depends upon the properties desired in the final product.

Selecting Silicones for Conditioning Shampoos

Figure 1 summarizes the variety of silicone materials available for use in conditioning shampoos. Cyclomethicone is the Cosmetic, Toiletry, and Fragrance (CTFA) designation for volatile cyclic silicones. These materials offer temporary conditioning and are generally used to formulate products with detangling properties.

Dimethicone, another methyl silicone, is available in a wide variety of viscosities and molecular weights. Dimethicones with viscosities less than 5 cSt are considered volatile; the most commonly used forms for personal care applications range from 350 cSt to 12,500 cSt. It is generally true that conditioning effects improve with increasing viscosity, but higher viscosities may be more difficult to formulate.

Two silicone "gum blends" were developed to offer a higher degree of conditioning to the hair and to make it feel more silky. These two silicones are known by their CTFA designations of:

- dimethicone (and) dimethiconol
- cyclomethicone (and) dimethiconol

These products are dispersions of very high molecular weight silicone gums in fluids of very low molecular weight dimethicone or cyclomethicone. The resulting

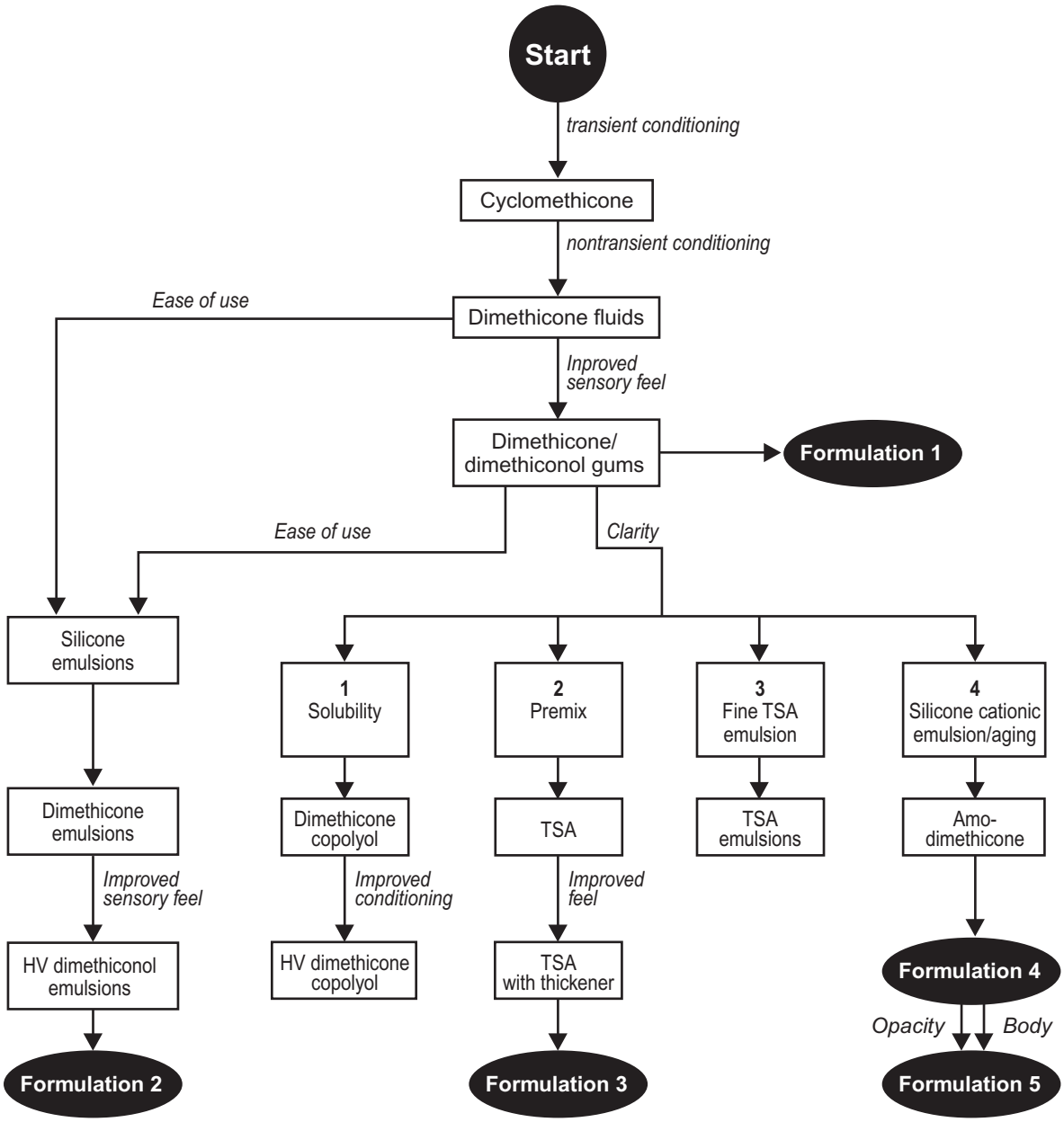

Figure 1. *Silicone selection guide for conditioning shampoos*

materials have viscosities in the range of 4,000 cP to 5,000 cP, and they are commonly used in the formulation of 2-in-1 conditioning shampoos. However, their use requires adherence to specific formulating techniques to ensure a stable emulsion.

The gum blends act as two-step conditioners. For example, in a formulation containing cyclomethicone (and) dimethiconol, the volatile cyclomethicone functions as a temporary conditioner. As it slowly evaporates, it improves the wet combing qualities of hair. The non-volatile dimethiconol acts as a permanent conditioner to provide improved dry combing and feel. Formulation 1 is an example of a product based on a silicone gum blend.

Silicone emulsions based on high molecular weight dimethicone or silicone gum blends have excellent compatibility in aqueous solutions, and they make hair silky and soft. In addition, these emulsions are easy to use, and they improve the dispersion of the silicone on hair. An example of this material has the proposed CTFA designation of dimethiconol (and) TEA-dodecylbenzenesulfonate. This silicone incorporates dimethiconol of more than 1 million cSt dispersed in a dodecylbenzene sulfonate detergent system. The final viscosity is 13 cSt,

Formulation 1. Prototype conditioning shampoo base formula using silicone gum blend.

Ingredient	Weight %
Phase A:	
1. Water	57.40
2. PEG-120 methylglucose dioleate	3.00
3. Sodium laureth sulfate	30.00
4. Cocoamidopropyl betaines	3.00
Phase B:	
5. Cyclomethicone (and) dimethiconol	2.60
6. Cocamide MEA	4.00
Phase C:	
7. Preservative	q.s.
8. Citric acid 50%	q.s.

Procedure: Combine ingredients of Phase A and heat to 60˚C. Combine ingredients of Phase B and heat to 60˚C. Add Phase B to Phase A and mix until uniform. Stir until mixture reaches room temperature. Add ingredient 7 and adjust the pH to approximately 6.5 with ingredient 8.

which makes the emulsion very easy to use. Formulation 2 is an example of the use of this silicone emulsion.

If the formulating objective is a transparent shampoo, dimethicone copolyol is an appropriate silicone selection, although its conditioning effect is not so strong as that achieved with silicone gum blends or aminofunctional silicone. However, dimethicone copolyol has been shown to reduce the eye irritation caused by sodium lauryl sulfate in the shampoo formulation.

Aminofunctional silicone incorporates an amino group within its Si-O structure. The essentially basic nature of the groups of primary amines causes this silicone polymer to develop a positive net charge in aqueous systems

Formulation 2. Prototype conditioning shampoo base formula using dimethiconol in detergent.

Ingredient	Weight %
1. Water	61.4
2. Acrylates/C_{10-30} alkyl acrylate crosspolymer	0.6
3. Ammonium lauryl sulfate	30.0
4. Cocamide DEA	3.0
5. Quaternium-60 (and) propylene glycol	0.5
6. Dimethiconol (and) TEA-dodecylbenzenesulfonate	4.0
7. Propylene glycol (and) diazolidinylurea (and) methyiparaben (and) propylparaben	0.5
8. Triethanolamine	q.s.
9. Ammonoim chloride	q.s.

Procedure: Heat water (ingredient 1) to 65˚C. Sprinkle in ingredient 2 while mixing, and mix until completely dissolved. Add ingredient 3; remove from heat and mix until uniform. Add ingredient 4, then ingredient 5, mixing well after each addition. When mixture is less than 40˚C, add ingredient 6. Add ingredient 7 and mix well. Adjust pH to 6 with ingredient 8. Adjust viscosity with ingredient 9 if necessary. This formulation is stable for more than 3 months at room temperature.

within a wide range of pH, ranging from 1 to 11.5. Therefore, aminofunctional silicone has great affinity with the hair, providing it with a considerable conditioning effect. This silicone family has broad application in hair treatments, especially when the hair is heavily damaged. Formulation 3 is an example of a formulation based on this type of silicone.

Emulsions based on aminofunctional silicones also have been developed, and these materials are especially useful for ease of formulation. For example, trimethylsily-

Formulation 3. Prototype conditioning shampoo base formula using aminofunctional silicone.

Ingredient	Weight %
1. Distilled water	63.25
2. Polyol alkoxy ester	1.50
3. Cocamide DEA	3.00
4. Trimethylsilylamodimethicone	2.00
5. Ammonium lauryl sulfate	30.00
6. DMDM hydantoin	0.25
7. 50% citric acid	q.s. to pH 6
8. Ammonium chloride	q.s.

Procedure: Combine ingredients 1 and 2; heat to 65˚C and agitate until uniform. Holding at 65˚C, add ingredients 3-5, mixing thoroughly after each addition. Cool to at least 35˚C and add water to replace volume. Add ingredient 6; mix until uniform. Adjust pH to 5.5 to 6 with ingredient 7. Measure viscosity and adjust with ingredient 8 (0.0 to 1.0%).

Formulation 4. Prototype clear shampoo base formula

Ingredient	Weight %
1. Water	45.30
2. Ammonium lauryl sulfate	48.00
3. Cocamide DEA	3.00
4. Amodimethicone (and) tallowtrimonium chloride (and) nonoxynol-10	2.00
5. Citric acid (50%)	q.s.
6. Ammonium chloride	0.50
7. Sodium chloride	1.00
8. Sodium laureth sulfate	0.20

Procedure: Combine ingredients 1, 2, and 3 with agitation until uniform. Add ingredient 4 with stirring. Adjust the pH to approximately 5 with ingredient 5. Add ingredient 6, then ingredient 7, both with agitation. Mix for several minutes, then add ingredient 8. Product will be slightly hazy.

lamodimethicone (and) Octoxynol-40 (and) isolaureth-6 (and) propylene glycol is a 35% nonionic emulsion of trimethylsilylamodimethicone, which is compatible with nonionic, cationic, and anionic systems. It disperses easily in water and provides effective wet and dry conditioning.

The final ingredient shown in the selection guide (Figure 1) is amodimethicone (and) tallowtrimonium chloride (and) nonoxynol-10. This emulsion is cationic and reactive, and it self-cross-links to form a conditioning film on the hair. The deposition effect can be controlled depending on the concentration of amodimethicone applied. This silicone is widely used in hair treatments, as well as in conditioning shampoos, in concentrations in the 0.5% range. Formulation 4 is an example of a formulation that incorporates this silicone; Formulation 5 is a pearlescent version that adds extra body.

Figure 2 compares improvements in wet combing contributed by various silicone materials, and Figure 3 shows the comparative durability of amodimethicone and dimethiconol on the hair.

Formulations based on anhydrous systems are primarily used as hair treatments and are applied to heavily damaged hair ends. In formulations of this type, (see Formulation 6) it is important to add the other non-aqueous ingredients (e.g., oils and other silicones) to the silicone gum blend instead of adding the gum blend to these other ingredients. This mixing order is necessary because the high molecular weight dimethiconol becomes very insoluble if added to the other materials.

Anhydrous formulations are very profitable for marketers, because material cost per ounce is very low in comparison to the price of the finished product in the marketplace.

Formulation 5. Prototype pearlized shampoo for body.

Ingredient	Weight %
1. Water	70.75
2. Sodium laureth sulfate	20.00
3. Sodium laureth sulfate (and) glycol stearate (and) cocamide DEA	5.50
4. Linoleic diethanol amide	3.50
5. Amodimethicone (and) tallowtrimonium chloride (and) nonoxynol-10	0.25
6. Citric acid 50%	q.s.
7. Sodium chloride	q.s.

Procedure: Dissolve ingredient 2 in ingredient 1, then add 3, 4 and 5 until dispersed. Adjust to pH 6.5 to 7.0 with ingredient 6 and add ingredient 7 to adjust viscosity.

Formulation 6. Treatment for heavily damaged hair.

Ingredient	Weight %
1. Cyclomethicone (and) Dimethiconol	90.0
2. Trimethylsilylamodimethicone	2.0
3. Cyclomethicone	9.0

Procedure: Mix ingredient 1 at medium speed with a moderate shear mixer. Slowly add ingredient 2 and continue mixing for 30 minutes after addition is complete. Slowly add ingredient 3. Continue mixing for 30 minutes after addition is complete. No heating is required.

Conclusions

A variety of silicone materials is available for use as conditioning agents in hair care products. These versatile ingredients have the tactile and aesthetic properties desired by consumers, and they can be formulated to provide high performance conditioning in shampoos and other hair treatments. In addition, in products such as anhydrous conditioners, silicones provide cost effective

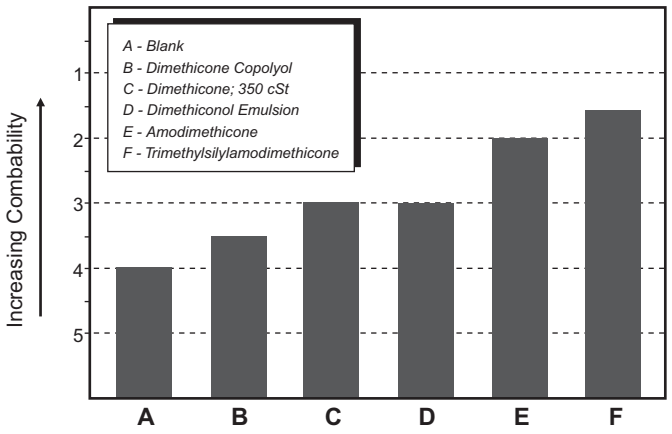

Figure 2. *Wet combing improvements in silicone-containing shampoos – initial evaluation.*

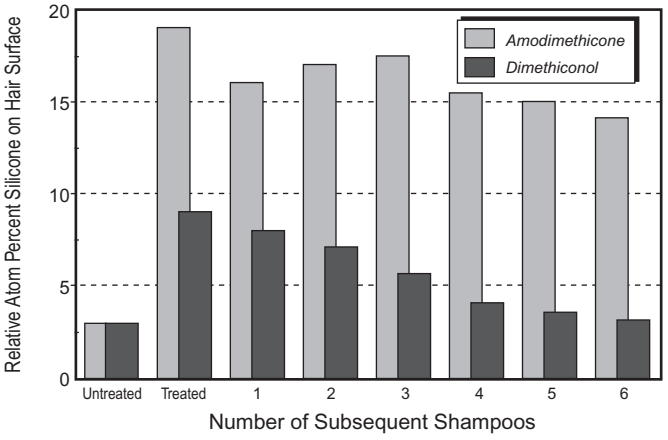

Figure 3. *Comparative durability of amodimethicone and dimethiconol on hair.*

conditioning for consumers combined with high profitability for marketers.

For Further Reading

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