

Selecting Silicone Surfactants for Personal Care Formulations

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ABSTRACT: *Interactions between a silicone surfactant and a fatty surfactant can alter the properties of a formulation. Here, the authors provide a case study of dimethicone copolyols in a shampoo.*

Silicone surfactants such as a dimethicone copolyol contain hydrophobic and hydrophilic portions enabling them to lower the surface tension of water.¹ The reduction of surface tension is a necessary first step in providing foam, emulsification, wetting and other surfactant properties. Each of these surfactant properties requires a molecule that lowers surface tension. Put another way, all molecules capable of foaming, emulsifying or wetting must be able to lower the surface tension, but not all molecules that lower surface tension provide these properties. The lowering of surface tension depends on the presence of hydrophilic and hydrophobic portions in the molecule. Additional surfactant properties depend on the structure of the molecule and its activity at the surface.

The function of dimethicone copolyol or any other silicone compound alone in aqueous solution may be of academic interest. However, it is of limited interest to a formulator because formulations are never simply water and dimethicone copolyol. The key to formulation is the interaction between the surfactants and other ingredients that alter the performance of the surfactants at the surface. There are interactions between different formulation components and understanding them and optimizing them for a given effect is key to formulation success.

This article is intended to educate cosmetic chemists in the chemistry of dimethicone copolyols and their potential effects in surfactant systems, such as shampoos or body washes. It will investigate some of the interactions between selected dimethicone copolyol compounds and a fatty surfactant and how they alter the properties of a solution or formulation.

The structures of materials chosen for evaluation are shown in **Figure 1**. Sodium lauryl sulfate (SLS) and sodium laureth-2 sulfate (SLES-2) were chosen because they are commonly used in personal care products. **Table 1** outlines the molecular weight information, the INCI name and the shorthand used to designate the compounds in this article.

Surface Tension in Aqueous Solutions

Aqueous solutions were prepared with the various materials at 1% by weight. The surface tension of each material was determined using a tensiometer^a.

Table 2 lists the results and clearly shows that the sulfated fatty alcohol

^a K100SF Tensiometer, Kruss GmbH

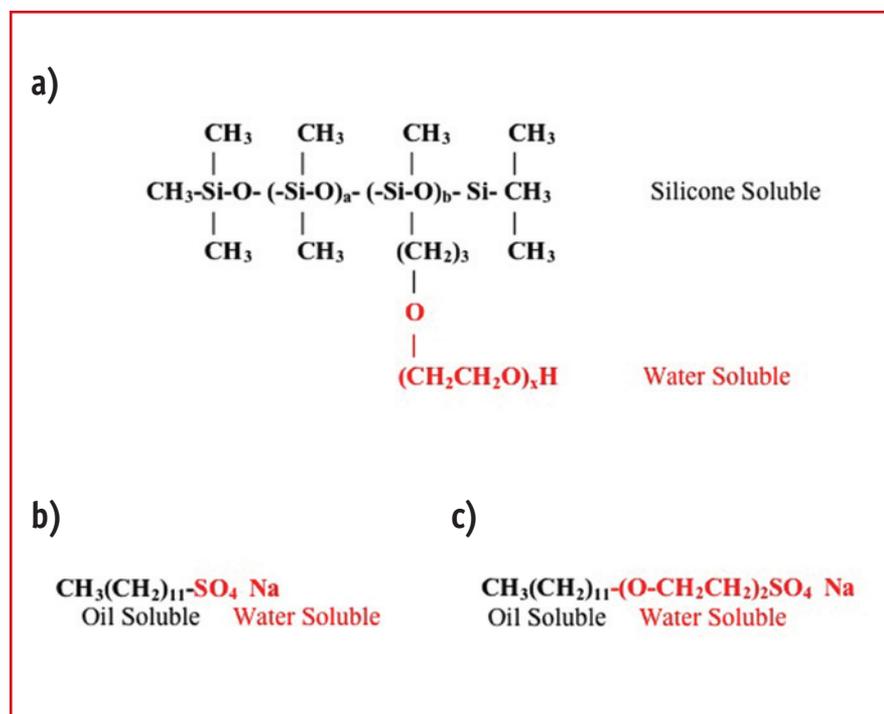


Figure 1. Compounds evaluated: a) dimethicone copolyol, b) SLS and c) SLES-2 sulfate

surfactants have a surface tension in the range of 30–32 dynes/cm². The silicone

surfactants have lower surface tension, in the range of 21–28 dynes/cm². The varia-

tion of surface tension within the class of silicone compounds is noteworthy. There has been a tendency to make generalizations that all silicone surfactants have essentially identical surface tension values. Clearly, this is not the case. As the silicone molecule contains less and less silicone, the surface tension becomes more like that of a fatty surfactant.

The surface tension is determined by the orientation of the surfactant molecule at the air/water interface. More specifically, surface tension is determined by the orientation of the organic functional groups on the surfactant molecule. These groups include silicon-containing portions, methyl groups, methylene groups and polyoxyalkylene groups. Action at the interface depends on the group that predominates at the surface when the molecule is in the lowest free energy conformation. The silicone portion of the molecule has an abundance of methyl groups, which makes the surface tension lower. The fatty surfactant groups have an abundance of methylene groups (-CH₂-), which makes the surface tension higher.

It is important to note that all silicone surfactants do not have the same low surface tension. Molecules that have long chains of ethylene oxide or propylene oxide have surface tensions like fatty surfactants, not silicone surfactants. As will be shown, the performance in formulations is complex; it depends upon the other components present.

Surface Tension in Binary Mixed Systems

Water is a unique material in that it orientates itself by hydrogen bonding. A hydrogen bond is a special type of dipole-dipole force that exists between an electronegative atom and a hydrogen atom bonded to another electronegative atom. Hydrogen bonding results in an orientation of molecules that have the lowest energy in the solution. This lowest energy state is favored. It results in the high surface tension of water. The reason oil and water separate from each other is that the two separate phases are at lower energy than when they are together. Simply stated, the number of hydrogen bonds between water molecules that need to be disrupted to keep oil in a water phase results in the separation of the phases being the lowest energy.

Table 1. Compounds evaluated

Material	Approx MW	INCI
SLS	320	Sodium lauryl sulfate
SLES-2	410	Sodium laureth-2 sulfate
DMC-1	700	PEG-8 dimethicone
DMC-2	5800	PEG-8 dimethicone
DMC-3	2500	PEG-8 dimethicone
DMC-4	1620	Bis-PEG-8 dimethicone

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Surfactants (fatty or silicone) experience hydrogen bonding in water. If there are several different surfactant types in water the interaction becomes more complicated albeit still driven by achieving the lowest energy.

The combination of SLS or SLES-2 with the various dimethicone copolyols suggests numerous possible interactions:

- Interactions from incompatibilities of the silicone, fatty and water-soluble domains in the surfactant. As with the oil and water interaction just described, these domains are incompatible with each other.
- Interactions from hydrogen bonding occurring between polyoxyalkylene domains of one molecule interacting with polyoxyalkylene domains or polar domains on another molecule. The nature of all of these interactions

collectively determines the surface tensions of the various blends.

DMC SLES-2 systems: Blends of SLES-2 at 95%, 90% and 50% with each DMC were prepared in solution with 1% of the blend and evaluated for surface tension. **Table 3** shows the results. Only DMC-1 had an impact on the surface tension of the solution. Of the four DMCs tested, DMC-1 had the lowest molecular weight. The interaction between the various functional groups in a formulation and the stability of the resulting complexes is critical to functionality of the formulation. If lowering surface tension is the goal of the addition, DMC-1 is the only DMC that will effectively accomplish the goal.

DMC SLS systems: Blends of SLS at 95%, 90% and 50% with each DMC were prepared in solution with 1% of the blend and evaluated for surface tension. **Table 3**

shows the results. As in the case of SLES-2, only DMC-1 had an impact, albeit slight, on the surface tension of the solution.

Foam and Wetting in Aqueous Systems

Table 4 shows the Draves wetting times for the neat surfactants at 1%

Table 2. Surface tension of selected materials at 1% in aqueous solution

Material	Dynes/cm ²
SLS	31.2
SLES-2	31.0
DMC-1	21.3
DMC-2	27.3
DMC-3	21.3
DMC-4	24.6

Table 3. Effect on surface tension, wetting and foam in 1% surfactant solutions when the surfactant is a blend of a dimethicone copolyol surfactant and a fatty surfactant, and the sulfate is 95%, 90% or 50% of the blend

Property	DMC	Fatty surfactant					
		SLES-2 95%	SLES-2 90%	SLES-2 50%	SLS 95%	SLS 90%	SLS 50%
	DMC-1						
Surface tension (dynes/cm ²)		30.3	29.9	26.7	30.3	30.0	28.1
Draves (sec)		4.0	4.4	5.3	3.5	3.0	7.7
Ross Miles (mm)							
Immediate		175	170	150	175	165	155
1 min		165	160	135	160	150	140
5 min		160	150	130	155	145	135
	DMC-2						
Surface tension (dynes/cm ²)		30.9	30.9	30.9	30.9	31.0	31.0
Draves (sec)		3.7	4.9	7.7	3.5	3.8	9.8
Ross Miles (mm)							
Immediate		185	180	150	170	170	160
1 min		170	170	140	150	150	140
5 min		160	160	135	145	150	135
	DMC-3						
Surface tension (dynes/cm ²)		30.6	30.6	30.6	31.0	30.9	31.0
Draves (sec)		4.5	4.6	12.9	3.7	4.8	14.3
Ross Miles (mm)							
Immediate		180	170	155	185	180	165
1 min		165	160	145	160	160	145
5 min		160	150	140	150	155	135
	DMC-4						
Surface tension (dynes/cm ²)		30.3	30.3	30.3	30.4	30.5	30.5
Draves (sec)		3.6	3.7	7.0	2.4	3.0	6.6
Ross Miles (mm)							
Immediate		170	170	145	180	180	150
1 min		150	155	120	155	160	135
5 min		140	150	40	145	155	130

Table 5. Draves wetting, Ross Miles foam and conditioning for dimethicone copolyol in a sodium laureth-2 sulfate shampoo (Formula 1)

Property	DMC-1	DMC-2	DMC-3	DMC-4
Draves (sec)	8.4	82.7	28.3	13.3
Ross Miles (mm)				
Immediate	115	105	100	120
1 min	110	95	80	115
5 min	110	85	65	105
Conditioning	1	4	3	2

Table 4. Draves wetting and Ross Miles foam for neat surfactants at 1% in water

Property	SLES-2	SLS	DMC-1	DMC-2	DMC-3	DMC-4
Draves (sec)	4.8	3.8	8.4	82.7	28.3	13.4
Ross Miles (mm)						
Immediate	170	180	115	105	100	120
1 min	155	165	110	95	80	115
5 min	150	150	110	85	65	105

in water. SLS and SLES-2 are both good wetting materials and good foaming compounds. DMC-1 is a good wetter and a fair foaming agent. DMC-2 and DMC-3 are neither good wetting agents nor good foaming compounds.

Foam and Wetting in Binary Mixed Systems

DMC and SLES-2 systems: Because SLES-2 is a high foaming surfactant, it was expected that the addition of DMC to SLES-2 would not improve foam. In fact, that is what happened. At concentrations of up to 10% added DMC, there was no negative effect upon foam or wetting with all blends of SLES-2. The foam was adversely effected with 50% added DMC. **Table 3** shows the results.

DMC and SLS systems: At all concentrations of added DMC, there was no negative effect upon foam or wetting with all blends of SLS. However, DMC-4 improved wetting in SLS systems.

Table 3 shows the result.

Simple Shampoo System

Materials and methods: The effect of DMC compounds on simple shampoos was studied using **Formula 1**.

The results are shown in **Table 5**. Conditioning on hair swatches was evaluated on a scale from 1 (worst) to 5 (best).

Results and discussion: The selection of a silicone to add to a shampoo formulation—even a very simple one—depends upon the effect desired. The appropriate silicone can be determined only in the formulation and can have no relationship to the properties of the silicone in solution alone.

Table 5 makes the following points for this simple formulation:

- For wetting effects, DMC-1 provides the best results;
- For foaming effects, DMC-4 provides the best results; and
- For conditioning effects DMC-2 provides the best results.

These results would not have been predicted from the data generated by evaluating either surfactant in water. The finished formula's raw materials, taken as a whole, are critical to determining the effectiveness of adding the silicone. There are significant interactions between surfactants in a formulation that alter the properties obtained when formulated together. The cosmetic formulation is more than merely the sum of its ingredients.

Formula 1. Simple shampoo

Water (<i>aqua</i>)	47.0% w/w
Sodium laureth-2 sulfate	40.0
Cocamidobetaine	10.0
Cocamid DEA	2.0
Dimethicone	<u>1.0</u>
	100.0

Conclusion

The selection of dimethicone copolyol for inclusion in hair care products is a complex process. The use of INCI names alone will be fruitless for picking the proper dimethicone copolyol for use in formulations. Likewise, the use of dimethicone copolyol's properties themselves in water to predict the functionality in formulation can be misleading. This is because there are various interactions between the dimethicone copolyol and the other surface active agents in the formulation. The formulation itself needs to be tested to determine if the formulation performs as desired.

The best test will be in the salon because in the final analysis consumer perception is the key to formulation performance. Dimethicone copolyols can be engineered to be formulator-friendly and provide the desired effect(s) in formulations.

It also needs to be noted that the compounds studied in this project are non-ionic silicone compounds, an important but limited class of materials. Improved conditioning can be obtained by working complexes of anionic and cationic silicones, designed specifically for that application.

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