 SCIENCE FOR FORMULATORS

Silicone Anionic / Silicone Cationic Complex Silicone Quaternium 20

Abstract The ability to formulate personal care products requires a chemist that not only understands the function of the various raw materials that are found in the formulation and the concentrations needed to be functional, the formulator must also understand that the interactions between the raw materials. The interactions can result in thickening, foam enhancement, aesthetics improvement and other desirable factors, however the interactions can cause instability, splitting, foam degradation and even loss of preservative functioning.

The ability to capitalize on interactions is not only of interest to the formulator; it is of interest to the raw material supplier as well. This article reviews the formation of silicone anionic and silicone cationic complexes and their functionality in formulation.

KEYWORDS: Silicone Complexes, Coacervate, Soft complexes, hard complexes, silicone quaternium 20, formulation iteraction, anionic / cationic interactions, shampoo, body wash, foam, aesthetics.

In a previous article on interaction between anionic and cationic surfactants, it is stated:
"The interaction between ingredients in a formulation is almost always the most important factor in determining the properties of the formulation (1). " The interaction between anionic and cationic surfactants are clearly one of the interactions that can be used to improve functional of a formulation. However, the ability to capitalize upon the interaction between anionic and cationic surfactants has been extended to anionic and cationic polymers and has been extended from formulators to raw material suppliers. This review article will address the development.

FORMULATOR TIP

The formulator should view old assumptions with a healthy degree of skepticism, understanding that assumptions sometimes, but rarely, are universally true; often contain an element of truth to them; and rarely are just wrong.

HARD AND SOFT COMPLEXES

Surfactant molecules interact with the solvent molecules around them. In order for a surfactant to be soluble in water, the surfactant molecules need to hydrogen bond with the water molecules. Ionic surfactants containing a charge, will be either positive or negative (Table 1).

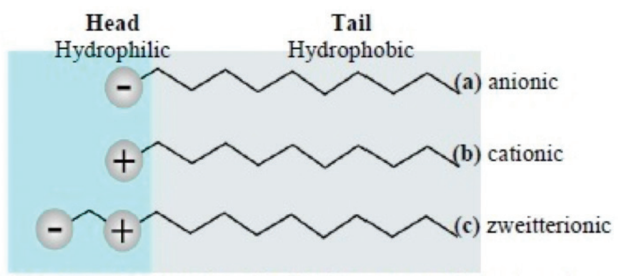

Table 1. Surfactant classification according to the composition of their head: a) anionic (negatively charged), cationic (positively charged) and c) zweitterionic (two oppositely charged groups).

Charges can increase the ability of forming hydrogen bonds with water molecules, however mixing ionic surfactants, it is important to consider the interactions of not only surfactant / water but also surfactant / surfactant interactions. When there is a mixture of positive and negative surfactants, the positive and negative chares on the surfactants can interact with one another. If the positive / negative interaction is strong (greater than the interaction of surfactant / water), the two surfactant molecules will prefer to interact with each other and not with the surrounding water molecules. This creates "shielding" of the charges from the water molecules and the surfactant can lose solubility in water. This is seen in Hard Complexes (HC) (3), the turbidity of the solution is

 SCIENCE FOR FORMULATORS

a result in the positive / negate interaction being stronger than the surfactant / water interactions (hydrogen bonds). As the solubility decreases, the particles start to scatter light leading to turbidity. The turbidity is clearly shown under laser light. If the positive / negative interaction is weak (less than the interaction of surfactant / water) the solution will remain clear and no surfactant precipitation will occur. This type of complex is referred to as Soft Complexes (SC) (3). The ability to formulate with SC materials provide the formulator with the ability to make unique formulations that can provide multifunctional properties. The difference between the two is shown in Table 2.

The difference between the two types of complex is the "solubility" of the particular anionic and cationic materials when paired up. It will be understood that when a blend of anionic and cationic surfactant is made, all ions of the combination dissociate in solution and the overall effect is a broad mix of the ions. Each will organize in the lowest free energy, and if that arrangement is soluble in water, a clear solution that does not disrupt a laser will occur.

The actual interaction between the various anionic and cationic species is quite complex and is shown graphically in Table 3 (4). The good news for the formulator is that the ability to use SC in formulation requires mixing the products and observing the clarity, not understanding all the possible interactions.

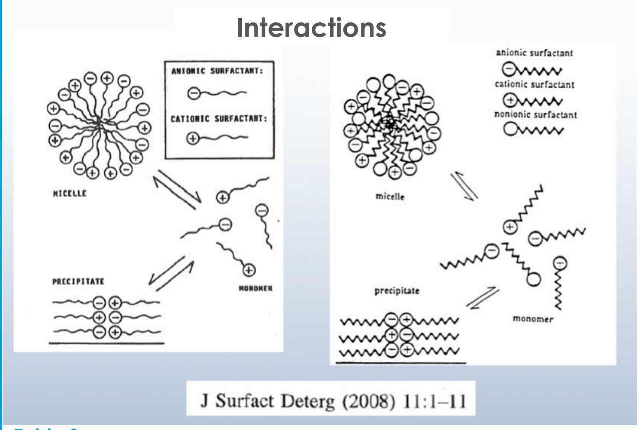

Table 3.

COMMERCIALLY AVAILABLE SOFT COMPLEXES

One commercially available soft complex (SC) is Silicone Quaternium 20. The structure is shown in Table 4. This material makes use of a silicone anionic and a silicone cationic that were specifically chosen to give an SC (soft complex).
There are several advantageous to using the complex over the cationic alone.

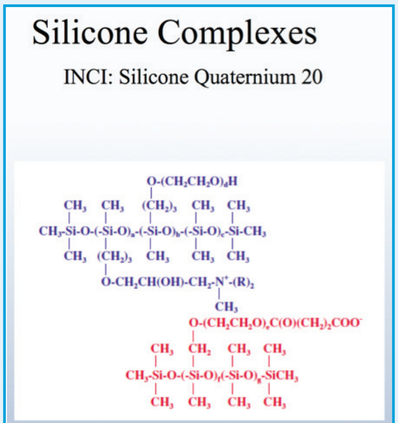

Table 4. Soft Complex Raw Material.

ANIONIC COMPATIBILITY

The complex can be added to anionic surfactant, like SLS or SLES maintaining clarity.

This can be easily shown with the following procedure:

- Prepare a 10% active solution of SLS or SLES-2
- Prepare a 10% active solution of Quat to be tested.
- Titrate 10% solution of Quat into 100 grams of 10% solution of anionic.
- End point is cloudiness or precipitate.

Incompatibility of quaternary compounds in anionic surfactants is a major problem when formulation personal care products. The limitations can be overcome by formulating with quats that have a greater compatibility with anionic surfactants as described in a previous article (1). Additionally, adding a cationic that has been complexed with an ionic before addition is another successful strategy to allow for incorporation of anionic and cationic surfactants together. Additionally, a particularly useful approach is to pre-combine a silicone anionic with a silicone cationic and subsequently add the complex to the surfactant system. In this case, the complex is silicone quaternium 20.

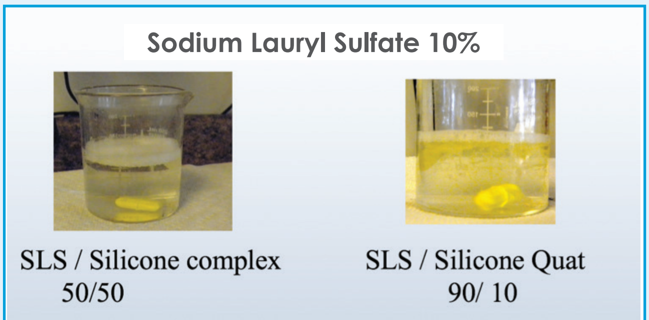

Table 5. shows that the silicone quaternary itself is not soluble in sodium lauryl sulfate, while the complex is soluble.

Note The SLS/Silicone complex is clear, while the incompatible SLS/ Quat in in two layers.

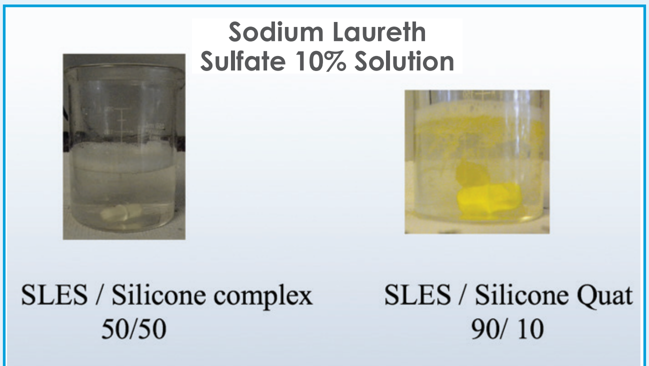

Table 6. Shows that the silicone quaternary itself is not soluble in sodium laureth sulfate, while the complex is soluble.

Note The SELS/Silicone complex is clear, while the incompatible SELS/ Quat in two layers.

COACERVATE SHAMPOO

Table 7 discloses a formulation for a coacervate (5) shampoo which demonstrates the effectiveness of using Silicone quaternium 20.

FORMULATOR TIP

An excellent article written by Robert Lochhead et al *entitled Deposition from Conditioning Shampoo: Optimizing Coacervate Formation* is recommended reading for all formulators interested in coacervate technology (7).

Procedure

1. Into a clean sanitized steel container equipped with a propeller mixer, add water in phase B.
2. Add SLES-2 and betaine in phase B and heat to 70-75C, slowly, adding cocamide MEA and EGDS. Mix slowly minimizing introduction of air. Mix until uniform then cool to room temperature.
3. In another clean sanitized steel container add the rest of the ingredients in phase A one by one while mixing and minimizing air entrainment.
4. Add phase B slowly into Phase A. Mix well until uniform.
5. Premix Silicone Quaternium 20 and Octyldodecyl citrate crosspolymer then add to premixed phase A and B.
6. Add the remaining Phase C under good agitation.
7. Add ingredients in Phase D, one by one. Adjust pH using citric acid to 5.5-6.5 and adjust viscosity to 6,000 to 12, 000 cps by addition of salt. Add fragrance.

2 in 1 Shampoo Coacervate

	Ingredient	% Wt
A		
	Water	22.00
	Acrylates Copolymer	2.50
	Triethanolamine	0.20
	Disodium EDTA	0.10
	Sodium Laureth 2 Sulfate	27.50
	Cocamido betaine	6.00
B		
	Water	18.00
	Sodium Laureth Sulfate	5.50
	Cocamido betaine	4.00
	Cocamid DEA	1.20
	Ethylene glycol distearate	3.00
C		
	Silicone Quaternium 20	1.00
	Octyldodecyl citrate crosspolymer	1.00
	Wheat Protein	0.50
	Cannabis Sativa Seed Oil	1.00
	DMDM Hydantoin	0.50
D		
	Decyl Glucoside	3.00
	Sodium Cocamphodiacetate	3.00
	Cirtric	Qs
	Sodium Chloride	Qs
	Fragrance	Qs
	Total	100.00

Table 7. Shampoo Formulation FH183D.

WET COMB

All products were evaluated on 10 inch Virgin Brown Hair. Two x 2 gram swatches were used for each test material, all from the same lot. All swatches were wet with water at 25oC and 1 gram of test material for each swatch. Swatches were washed and then rinsed for one minute per swatch. Wet comb evaluation was then performed. Hair was not blow dried, rather they were air dried.

Evaluation scale 1 -5. (1 worst – 5 best) Table 8 shows the results.

A well-known baby shampoo was also evaluated.

	Wet Comb	Rinse off	Clean Feel	Shine	Residual Feel
Water only	1.0	3.0	2.0	2.0	2.0
Baby Shampoo	2.0	3.0	3.0	2.0	2.0
FGH183D	4.5	4.5	4.5	3.0	3.0

Table 8. Wet Comb Analysis.

Table 9 shows the results for dry comb analysis.

	Dry Comb	Dry Feel	Clean Feel	Shine	Manageability	Fly Away	Residual Feel	Static
Water only	3.0	3.0	2.0	1.0	1.0	1.0	1.0	2.0
Baby Shampoo	3.0	3.5	3.0	1.0	2.0	2.0	1.0	2.0
FGH183D	4.5	3.5	4.0	4.0	4.0	4.0	4.0	4.0

Table 9. Dry Comb Analysis.

FORMULATOR TIP

Always look at new ways to combine old ingredients to solve formulation problems and to introduce new formulation aesthetics. These should include differing ratios of ingredients, different orders of addition, and different combinations. Remember, the interactions that are observed in our formulations are complex and not necessarily well understood.

CONCLUSIONS

1. Silicone Quaternium 20 is an outstanding additive to a variety of shampoo systems. When added to baby shampoo at a level of between 0.5 and 0.75% by weight the shampoo exhibits outstanding conditioning effects without sacrificing the sting free, and eye irritation claims. In short, the product is transformed into a family shampoo.
2. Silicone Quaternium 20 is an outstand product for heavy full hair, especially Asian, African American and Latino hair. It provides softness, combability and shine to the hair.
3. Silicone Quaternium 20 is non-irritating the eyes, unlike many fatty quats.
4. Silicone Quaternium can be used in body wash applications where it provides a very pleasant aesthetic to the skin.
5. Finally, Silicone Quaternium 20 can be used to make coacervate delivery systems.

REFERENCES AND NOTES

1. O'Lenick, Tony , H&PC Today - Household and Personal Care Today, vol. 11(4) July/August 2016 p,10-12
2. https://fouling-on-solar-panels.wikispaces.com/Solutions+Surfactants
3. O'Lenick, Tony HPC Today - Household and Personal Care Today, vol. 11(3) May/June 2016 p 37-40
4. O'Lenick, Tony Cosmetics and Toiletries , Vol. 120 No. 11 November 2005 p. 63-64.
5. The term "coacervate" refers to spherical aggregates of colloidal droplets held together by hydrophobic forces. Coacervate droplets can measure from 1 to 100 micrometres across, while their soluble precursors, are typically on the order of less than 200 nm (6).
6. https://en.wikipedia.org/wiki/Coacervate
7. Lochhead, Robert, Huisings Lisa and Waller Tara. Cosmetics and Toiletries Vol. 121, No. 3/March 2006.

About the author

TONY O'LENICK
Siltech L.L.C., Lawrenceville, USA