PEG Dimethicone in Shampoos

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KEYWORDS: PEG Dimethicone, shampoo, wet combing, dry combing, foam, terminal polymer, comb polymer, star polymer, greening with silicones.

ABSTRACT

Within the group of what are called "Silicone polymers" are a large group of related polymers that have many different functionalities. One of the most interesting are a class of polymers that are "hybrid" or "organofunctional" polymers. It is this group of surface active polymers that have at least two functional groups that are not soluble in each other in pure form. These groups include silicone soluble, oil soluble, water soluble and fluoro-soluble.

This article deals with a class of compounds with the INCI name of PEG/PPG dimethicone. They contain a hydrophilic group that allows for improves solubility. Within this group are compounds that are water soluble and non-ionic. These can be easily formulated into shampoos and other water-based products to provide surface tension reduction, foam and wet comb. Unlike cationic silicones, PEG dimethicone polymers are compatible with anionic surfactants and can easily improve the properties of simple shampoos. This article deals with several classes of PEG dimethicone polymersd structures including, comb polymers, terminal polymers and star polymers.

Silicone polymers are chosen for formulations to fulfil a basic need that cannot be achieved using other chemistries. Silicone polymers have a handful of salient properties that make them valuable in formulations.[1] These properties are outlined in Table 1.

A properly closed silicone polymer can provide the following attributes to formulations;

1. Lowering surface tension to around 25 dynes/cm
2. Providing unique skin feel, cushion and playtime
3. Providing unique solubilities (are soluble in silicone, oil, water and fluoro compounds)
4. Can provide emulsification with unique aesthetics (especially invert emulsions
5. Provide film/formation
6. Provide water resistance
7. Provide foaming for non-traditional formulations

FORMULATOR TIP

While it is true that silicones can provide the 7 attributes, it is highly unlikely that a single PEG dimethicone can provide ALL of the attributes. The formulator is challenged to look at the variety of materials available and to determine which of these attribute(s) are provided by a particular silicone polymer. Such an understanding will make development in the future easier once the structure/ function relationships are known.

GREENING WITH SILICONES[2]

Recently, silicone polymers have come under increased scrutiny. One simplistic approach, favored by some, is the complete banning of all raw materials that do not meet a specific definition of green, including silicones. This approach, while simple, fails to consider the fact that successful products need to have the proper combination of consumer and environmental acceptability. Simply put, consumers will not wash their hair with simple soap despite it being green, because it lacks many other attributes demanded by the consumer. The other approach is to simply accept all products regardless of ingredients.

The approach that appears to offer the best possibility is the so-called Hybrid Formulation Model. This approach compares the cosmetic formulation to the hybrid car and speculates that the optimized consumer product is one that will be as green as the category can be (the electric part), while using a minimal quantity of materials that are not green only in special instances where performance

demands it (the gasoline portion). This approach results in a metric system, referred to as the Green Star System, that allows one to consider both the environmental and performance aspects of the product. This concept encourages the use of minimal concentrations of raw materials that offer unique consumer benefit while keeping the green aspect uppermost in formulations. The result is a process as much as a product. The process is one of continuous re-evaluation of formulations ever increasing the green efficiency of raw materials.
We recommend that silicone polymers be limited to 10% maximum in formulations, relying upon organic sustainable materials to provide most of the desired properties. This study we add 2% by weight of PEG Dimethicone to formulation.

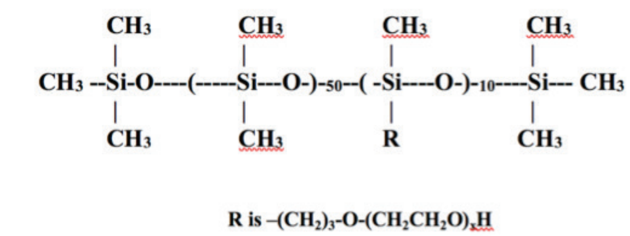
FORMULATOR TIP

Silicone polymers are specialty materials. They are quite costly and therefore their use in formulation requires the level used to be very low. Always look at the cost per unit formulation, not just the cost per pound of raw material. Once you believe the formulation has been optimized, lower the concentration by 30%. See if there is a change. If a formulation is compared to a gourmet meal, silicones will be the spice, not the meat and potatoes.

PEG DIMETHICONE

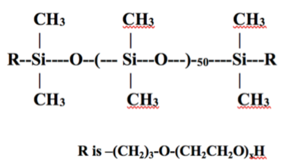
What distinguishes PEG/PPG Dimethicone polymers from other classes of compounds is the presence of the hydrophilic water loving PEG/PPG group.[3] There are three distinct structures for PEG/PPG Dimethicone molecules Comb Structures (Structure 1) in which the PEG/PPG group in only internal, Terminal Structures (Structure 2) in which the PEG/PPG groups are only at the ends and finally Star Structures (Structure 3) in which the PEG/PPG groups are in both positions.[4,5] It is the structure and the % by weight of the polymer that in large part determines the functionality in formulation.

Comb Structure 1.

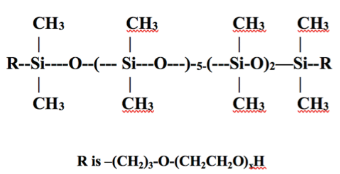


This study will include candidates with each type of structure and have enough PEG to render the molecule water soluble. Table 2 shows the PEG Dimethicone polymers studied.

Terminal Structure 2.



Star Compound Structure 3.



INCI Name	DMC	% EO	MW	Type
PEG 12 Dimethicone	A	62	3414	Comb (Structure 1)
PEG 8 Dimethicone	B	69	2042	Comb (Structure 1)
Bis PEG 10/10 Dimethicone	C	62	4021	Star (Structure 3)
Bis PEG 10 Dimethicone	D	48	1850	Terminal (Structure 2)

Table 2. Compounds Studied.

SHAMPOO

In order to understand the function of PEG Dimethicone in shampoo systems, a simple formulation was chosen to minimize the effect of other additives.

Shampoo Base (Sil-SP-0003) and with 2% of PEG Dimethicone:
Table 3 shows a clear 2 in 1 shampoo formulation (Sil-SP-0003).

Formula No.	Sil-SP-0003	Sil-SP-0003a	Sil-SP-0003b	Sil-SP-0003c	Sil-SP-0003d
Ingredients	**Weight %**	**Weight %**	**Weight %**	**Weight %**	**Weight %**
Phase A: D.I. Water	52.45	50.45	50.45	50.45	50.45
SLES-2	35	35	35	35	35
Cocamidopropyl Betaine	7	7	7	7	7
Cocoamide DEA	4	4	4	4	4
Disodium EDTA	0.1	0.1	0.1	0.1	0.1
DMDM Hydantoin	0.7	0.7	0.7	0.7	0.7
Phase B: Sodium Chloride	q.s.	q.s.	q.s.	q.s.	q.s.
Citric Acid (40% aq)	0.75	0.75	0.75	0.75	0.75
A	0	**2**	0	0	0
B	0	0	**2**	0	0
C	0	0	0	**2**	0
D	0	0	0	0	**2**
Total	100	100	100	100	**100**

Table 3. (Clear 2 in 1).

All formula pH adjustments ranged from 4.5 to 5.5, same as natural 'pH' of our hair and skin.

Procedure:

1. Into a clean and sanitized stainless steel tank equipped with a propeller mixer, sift into water, and then add the rest of ingredients one by one slowly in Phase A while minimizing air incorporation.
2. Adjust pH by using citric acid to pH = 4.5 ~ 5.5, and adjust viscosity to 3,600 cps ~ 12, 000 cps by addition of NaCl (q.s.).

Formula No.	FH181	FH181A	FH181B	FH181C	FH181D
Ingredients	**Weight %**	**Weight %**	**Weight %**	**Weight %**	**Weight %**
Phase A: D.I. Water	21.3	19.3	19.3	19.3	19.3
Carbopol Aqua SF-1	3	3	3	3	3
TEA (99%)	0.2	0.2	0.2	0.	0.2
Na_2EDTA	0.1	0.1	0.1	0.1	0.1
SLES-2	28	28	28	28	28
Cocamidopropyl Betaine	6	6	6	6	6
Decyl Glucoside	4	4	4	4	4
Disodium Cocoamphodiacetate	4	4	4	4	4
Phase B: D.I. Water	18	18	18	18	18
SLES-2	5.5	5.5	5.5	5.5	5.5
Cocamidopropyl Betaine	4	4	4	4	4
Cocamide DEA	1.2	1.2	1.2	1.2	1.2
Ethylene Glycol Distearate	3	3	3	3	3
Phase C: Wheat Protein	0.5	0.5	0.5	0.5	0.5
DMDM Hydantoin	0.7	0.7	0.7	0.7	0.7
Phase D: Sodium Chloride	q.s.	q.s.	q.s.	q.s.	q.s.
Citric Acid (40% aq)	0.5	0.5	0.5	0.5	0.5
DMC A	0	**2**	0	0	0
DMC B	0	0	**2**	0	0
DMC C	0	0	0	**2**	0
DMC D	0	0	0	0	**2**
Total	100	100	100	100	100

Table 4. Formulations for Opaque Shampoo Base (FH 181) and with 2 % of DMC.

Table 4 shows an opaque conditioning shampoo (FH181).

Procedure:

1. Into a clean and sanitized stainless steel container equipped with propeller mixer, sift into water in Phase B and SLES-2 and Betaine, heat up to 50 to 60 °C, slowly add Cocamide MEA and EGDS, mix slowly while minimizing air incorporation. Mix until uniform, then cool down to room temperature.
2. In another clean and sanitized stainless steel tank equipped with propeller mixer, sift into water and add the rest of ingredients one by one in Phase A while minimizing air incorporation. Mix until uniform.
3. Add phase B slowly into Phase A. Mix until uniform.
4. Add ingredients one by one of Phase C into Phase A+B while minimizing air incorporation.
5. Add silicone polyether, mix well, then adjust pH by using citric acid to pH = 5.5 ~ 6.5, and adjust viscosity to 3,600 cps ~ 12,000 cps by adding NaCl (q.s.).

Table 5 shows the results of analysis performed on the shampoo formulations.

Formula	pH	Viscosity (cps) (Brookfield LVT #4, 12 rpm)	Appearance	Stability @ 50°C
Sil-SP-0003 **(Control)**	5.16	12,000 (+0.5% NaCl)	Clear gel	Stable for 2 weeks
Sil-SP-0003a **(DMC A)**	5.02	4,600 (+1% NaCl)	Clear gel	Stable for 2 weeks
Sil-SP-0003b **(DMC B)**	4.67	100 (no NaCl added) 3,600 (+ 2% NaCl + 2% Crothix®*)	Clear gel	Stable for 2 weeks
Sil-SP-0003c **(DMC C)**	5.04	900 (no NaCl added) 12,000 (0.5% NaCl)	Clear gel	Stable for 2 weeks
Sil-SP-0003d **(DMC D)**	4.98	500 (no NaCl added) 12,000 (+ 0.2% NaCl)	Clear gel	Stable for 2 weeks

Table 5. Analysis Clear Shampoo.

* Crothix® is PEG-150 Pentaerythrityl Tetrastearate (and) PEG-6 Caprylic/Capric Glycerides (and) Water

From Table 5, The effectiveness of salt in increasing viscosity was , Sil-SP-0003D > C > A > B.

Table 6 shows the results of analysis performed on the opaque shampoo formulation.

Formula	pH	Viscosity (cps) (Brookfield LVT #4, 12 rpm)	Appearance	Stability @ 50°C
FH181 (Control)	5.84	11,000 (no NaCl added)	Opaque white cream	Stable for 2 weeks
FH181A (DMC A)	6.01	10,000 (no NaCl added)	Opaque white cream	Stable for 2 weeks
FH181B (DMC B)	5.88	500 (no NaCl added) 2,200 (+1% NaCl)	Opaque white cream	Stable for 2 weeks
FH181C (DMC C)	5.88	1500 (no NaCl added) 9,000 (+1% NaCl)	Opaque white cream	Stable for 2 weeks
FH181D (DMC D)	6.16	3,700 (no NaCl added)	Opaque white cream	Stable for 2 weeks

Table 6. Analysis Opaque Shampoo.

From Table 6, The effectiveness of salt in increasing viscosity was FH181A/C/B/D.

FOAM EVALUATION

Method 1. All products were evaluated with the same procedure. A 500 mL cylinder with 2 mL increments with glass stopper was used. All samples and distilled water was prepared at 25 °C. 1.00 gram of test material was used, and 100 mL distill water was added to dissolve the test material in a 250 mL beaker. After the test material was totally dissolved, the solution was transferred into the cylinder, then shaken in the left and right direction, 10 shakes to the left, and 10 shakes to the right. Then back and forth direction, 10 shakes to the forth, and 10 shakes to the back. Each test material had an "Initial" reading and then a "2 minute" reading and their Foam Height were documented. Each material was evaluated 3 times and their averages were documented. The scale for Foam Height is 500 mL is outstanding and 100 mL is very poor. The type of foam was also noted whether it is tight or loose. All shakes were done manually.

In order to get more information about the foam height of test materials, another method also used to evaluate their foaming potential.

Method 2. All products were evaluated with the same procedure. A 1000 mL cylinder with 10 mL increments was used. All samples and distilled water was prepared at 25 °C. 1.00 gram of test material was used, and 100 mL distill water was added to dissolve the test material in a 250 mL beaker. After the test material was totally dissolved, the solution was transferred into the cylinder. An outlet of air pump was placed on the bottom of the cylinder to generate the bubbles. Record the foam height within 20 seconds for each test materials, each material was evaluated 3 times and their averages were documented.
The scale for Foam Height is 1000 mL is outstanding and 100 mL is very poor. The type of foam was also noted whether it is tight or loose. Bubbles were generated by electronic air pump.

Table 7 shows the results using Method 1 for the foam of the clear shampoo.

Sample	**Initial Reading** (average)	**Two Minute Reading** (average)
CAB (Cocamidopropyl Betaine)	300	270
Sil-SP-0003 (Control)	247	242
Sil-SP-0003a (DMC A)	247	242
Sil-SP-0003b (DMC B)	237	228
Sil-SP-0003c (DMC C)	252	245
Sil-SP-0003d (DMC D)	275	265

Table 7. Foam Height (Measured by Method 1).

Table 8 shows the results using Method 1 for the foam of the opaque shampoo.

Sample	Initial Reading (average)	Two Minute Reading (average)
FH 181 (Control)	265	255
FH 181A (DMC A)	265	260
FH 181B (DMC B)	260	255
FH 181C (DMC C)	270	265
FH 181D (DMC D)	280	275

Table 8. Foam Height (Measured by Method 1).

All foams were tight and uniform.

Table 9 shows the foam data using Method 1 on both shampoos studied.

Table 10 shows the foam height using Method 2 on the clear shampoo.

Table 11 shows the foam height using Method 2 on the opaque shampoo.

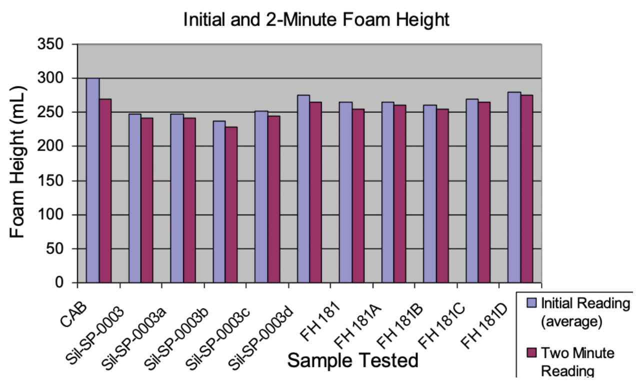


Table 9.

Sample (Bubble for 20 sec)	Initial Reading (average)	Two Minute Reading (average)	Five Minute Reading (average)
CAB (Cocamidopropyl Betaine)	650	630	600
Sil-SP-0003 (Control)	710	700	680
Sil-SP-0003a (DMC A)	700	690	670
Sil-SP-0003b (DMC B)	655	640	620
Sil-SP-0003c (DMC C)	690	680	660
Sil-SP-0003d (DMC D)	680	670	650

Table 10. Foam Height (Measured by Method 2.).

Sample (Bubble for 20 sec)	Initial Reading (average)	Two Minute Reading (average)	Five Minute Reading (average)
FH 181 (Control)	685	670	650
FH 181A (DMC A)	690	680	660
FH 181B (DMC B)	680	670	650
FH 181C (DMC C)	675	660	640
FH 181D (DMC D)	680	670	650

Table 11. Foam Height (Measured by Method 2.).

All foams were tight and uniform.

Table 12 shows the foam height using Method 2 on both shampoos in graphic form.

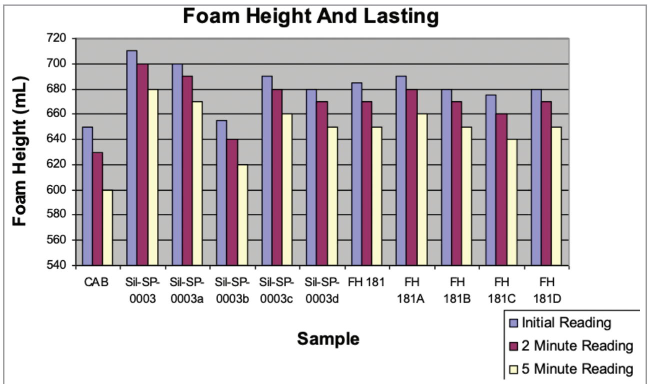


Table 12. Method 2.

From above data, we can see that DMC B has the lowest foam height, and DMC A has the highest foam height in formulas Sil-SP-0003, but the results can be modified with other ingredients; these can be seen from formulas FH181A/B/C/D.

RAW MATERIAL FOAM

In order to get more detail information about foam potential of DMC materials, 1 gram of each material [CAB, DMC A, DMC B, DMC C, DMC D, and SLES-2 (25%)] was dissolved in 100 grams of D.I. water, and the foam height measurements by method 2 were listed in Table 13.

Sample (Bubble for 20 sec)	Initial Reading (average)	Two Minute Reading (average)	Five Minute Reading (average)
CAB	650	630	600
DMC A	685	660	630
DMC B	620	590	540
DMC C	640	610	570
DMC D	605	520	400
SLES-2	690	670	650

Table 13. Raw Material Foam Data.

Table 14 shows the foam heights of the raw materials.

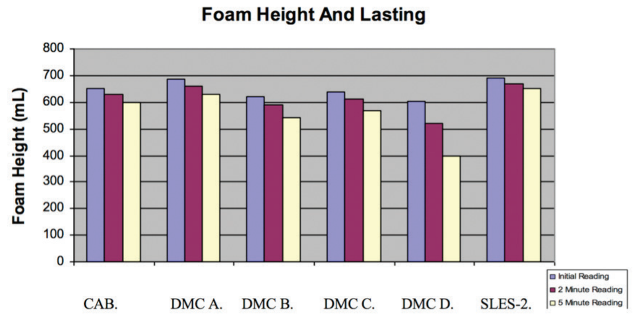


Table 14. Foam of Raw Materials.

Foams of CAB, DMC B, DMC C, SLES-2 were uniform and tight, but foams of DMC B, and DMCA were loose. Again, DMC A is the most foam potential silicone polyether in the test materials.

HAIR EVALUATION:

All products were evaluated on 10-inch Virgin Brown Hair. Two x 2-gram swatches were used for each material tested, all from the same lot. All swatches were wet with 25 °C water and one gram of test material was used for each swatch. Swatches were washed and then rinsed for at least one minute per swatch. Wet Comb Evaluation was then performed. No blow-drying of hair was done. All swatches air-dried then the Dry Comb Evaluation was performed once hair was completely dry.

Scale used is 1 to 5, 5 being the best. Used for wet and dry combing. Table 15 shows wet comb data for the clear shampoo and Table 18 shows the wet comb for the opaque shampoo.

	Wet Comb	Rinse off	Clean Feel (Scroop)	Shine	Residual Feel	Average
Control Water only	1	3	2	2	2	2
Sil-SP-0003 (Control)	2.5	3.5	3.5	3	3	3.1
Sil-SP-0003a (DMC A)	3.5	3.5	3.5	3	3	3.3
Sil-SP-0003b (DMC B)	3	3.5	3.5	3	3	3.2
Sil-SP-0003c (DMC C)	3.5	4	4	3	3	3.5
Sil-SP-0003d (DMC D)	3	3.5	3.5	3	3	3.2

Table 15. Wet Combing Evaluation Clear Shampoo.

	Wet Comb	Rinse off	Clean Feel (Scroop)	Shine	Residual Feel	Average
FH 181 (Control)	3	4	4	3.5	3.5	3.6
FH 181A (DMC A)	3.5	4	4	3.5	3.5	3.7
FH 181B (DMC B)	3	4	4	3.5	3.5	3.6
FH 181C (DMC C)	3.5	4.5	4.5	3.5	3.5	3.9
FH 181D (DMC D)	3	4	4	3.5	3.5	3.6

Table 16. Wet Combing Evaluation Opaque Shampoo.

	Dry Comb	Dry Feel	Clean Feel /Look	Shine	Fullness/ Manageable	Flyaway	Residual Feel	Static	Average
Control Water only	3.0	3.0	2.0	1.0	1.0	1.0	1.0	2.0	1.75
Sil-SP-0003 (Control)	3.5	3.5	3.5	3.0	3.5	3.0	2.5	3.0	3.19
Sil-SP-0003a (DMC A)	3.5	3.5	3.5	3.0	3.5	3.0	2.5	3.0	3.19
Sil-SP-0003b (DMC B)	3.5	3.5	3.5	3.0	3.5	3.0	2.5	3.0	3.19
Sil-SP-0003c (DMC C)	4.0	3.5	3.5	3.0	3.5	3.0	2.5	3.5	3.31
Sil-SP-0003d (DMC D)	4.0	3.5	3.5	3.0	3.5	3.0	2.5	3.0	3.25

Table 17. Dry Combing Evaluation Clear Shampoo.

Table 17 shows dry comb data for the clear shampoo and Table 20 shows the dry comb for the opaque shampoo.

	Dry Comb	Dry Feel	Clean Feel /Look	Shine	Fullness/ Manageable	Flyaway	Residual Feel	Static	Average
FH 181 (Control)	4.0	4.0	4.0	3.5	4.0	3.5	3.0	3.5	3.69
FH 181A (DMC A)	4.0	4.0	4.0	3.5	4.0	3.5	3.0	3.5	3.69
FH 181B (DMC B)	4.0	4.0	4.0	3.5	4.0	3.5	3.0	3.5	3.69
FH 181C (DMC C)	4.0	4.0	4.0	3.5	4.0	3.5	3.0	4.0	3.75
FH 181D (DMC D)	4.0	4.0	4.0	3.5	4.0	3.5	3.0	3.5	3.69

Table 18. Dry Combing Evaluation Opaque Shampoo.

We can conclude from Tables 15-18 and Table 6 that DMC C is the best for wet and dry combing evaluation. DMC D and DMC A also can be a good candidate for shampoo formulation. If using DMC B, one should be very careful to use something other than salt to build viscosity.

SALT TOLERANCE, PH, VISCOSITY, EASE OF FORMULATION, EFFECT ON FORMULATION STABILITY

Scale used is 1 to 5, 5 being the best, only for salt tolerance, Ease of formulation, effect on formulation stability. Viscosity was tested by using Brookfiled, LVT, #4 spindle, 12 rpm. Table 19 shows the results for the clear shampoos and Table 20 shows the results for the opaque formulation. These table give a good overview of the properties of the formulations.

Clear Shampoo

Evaluation / Formula	Salt Tolerance	pH	Viscosity, cps (NaCl added with*)	Ease of Formulation	Effect on formulation Stability	Average
Sil-SP-0003 (Control)	1.5	5.16	1000 12,000* (0.5% NaCl added)	3.0	3.5	2.67
Sil-SP-0003a (with DMC A)	3.0	5.02	200 4,600* (1% NaCl added)	4.0	4.0	3.67
Sil-SP-0003b (with DMC B)	3.5	4.67	100 2, 000* even add 2% NaCl	3.0	3.0	3.50
Sil-SP-0003c (with DMC C)	2.5	5.04	900 12000* after adding 0.5% NaCl	4.5	4.5	3.83
Sil-SP-0003d (with DMC D)	2.5	4.98	500 22,000* after adding 0.4% NaCl	4.0	4.5	3.67

Table 19. Evaluation of Salt tolerance, pH, Viscosity, Ease of formulation, Effect on formulation Stability.

CONCLUSIONS

The ability to formulate interesting properties into a shampoo by simply adding 2% by weight of a PEG dimethicone offers the formulator the possibility of making a variety of products offering the market very different consumer perceptible possibilities. The non-ionic nature of these PEG dimethicone polymers and their the compatibility in water soluble systems allows for simple additions to formulations.

Opaque Shampoo

Evaluation / Formula	Salt Tolerance	pH	Viscosity, cps (NaCl added with*)	Ease of Formulation	Effect on formulation Stability	Average
FH181 (Control)	1.0	5.84	11,000	3.0	3.5	2.50
FH181A (with DMC A)	1.5	6.01	10,000	4.5	4.5	3.50
FH181B (with DMC B)	3.0	5.88	2, 200* (1% NaCl added)	3.5	3.5	3.33
FH181C (with DMC C)	2.5	5.88	9,000* (1% NaCl added)	4.5	4.5	3.83
FH181D (with DMC D)	2.5	6.16	3,700	4.5	4.5	3.83

Table 20. Evaluation of Salt tolerance, pH, Viscosity, Ease of formulation, Effect on formulation Stability.

The ability to get acceptable foam, conditioning, scroop control and good wet and dry comb is quite attainable. DMC A, DMC C and DMC D are all good candidates with some differences in properties.

DMC C is very interesting as it is a relatively new material[4,5] and has great conditioning abilities with good to outstanding other properties in formulation.

While interesting, DMC B is different from other three candidates, requiring one should use caution on the viscosity when apply it in shampoo.

This study was conducted with fairly simple formulations. The formulator will be able to make changes to the formulation to maximize performance and minimize cost.

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