Analysis of volatile dimethicones for cosmetics

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Volatile linear silicones are low molecular weight fluids (varying from 0.65 cSt to 2 cSt) which are excellent clear odourless emollients for personal care.

Volatile on skin, they present low surface tension, fast rate of evaporation, unique lubricity, ability to spread easily and good miscibility with most of ingredients (see Table 3). As a result, they are exceptional silky and non-greasy carriers for skin care, deodorant and antiperspirants, sun care, hair care and colour cosmetics.

For instance, in makeup they act as a volatile carrier in pigment dispersions, in aerosols they can be used as a replacement for organic solvents, while in sun care they can be used as a solvent for actives and a dispersing aid for micronised oxides.

Upon evaporation, volatile linear silicones impart soft, dry velvety feel, with no residue or build-up. They reduce stickiness, and as a result in sprayable formulations they reduce clogging of nozzles. In stick formulations they are non-tacky, and can be applied without drag, and emulsions are soft, with a smooth feel and pleasant application with a unique skin-feel.

In order to manufacture low viscosity dimethicones, BRB use a novel process to polymerise siloxanes with negligible D4 content.

The carbon footprint being minimal in the procedure is a step forward towards BRB's commitment to develop and use eco-friendly processes.

Further to polymerisation, the product is distilled in several tall continuous distillation columns to obtain silicones of extremely high purity.

Figure 1: Distillation unit in Malaysia plant.

Flawless sensory

As we have observed in Table 3, super low viscosity dimethicones present better compatibility with most cosmetic ingredients compared to low viscosity classical dimethicones (from 5 cSt-20 cSt).

A wide palette of silicone volatile linear fluids is available on the market to achieve superior sensory. Figure 2 illustrates volatility of different low viscosity fluids.

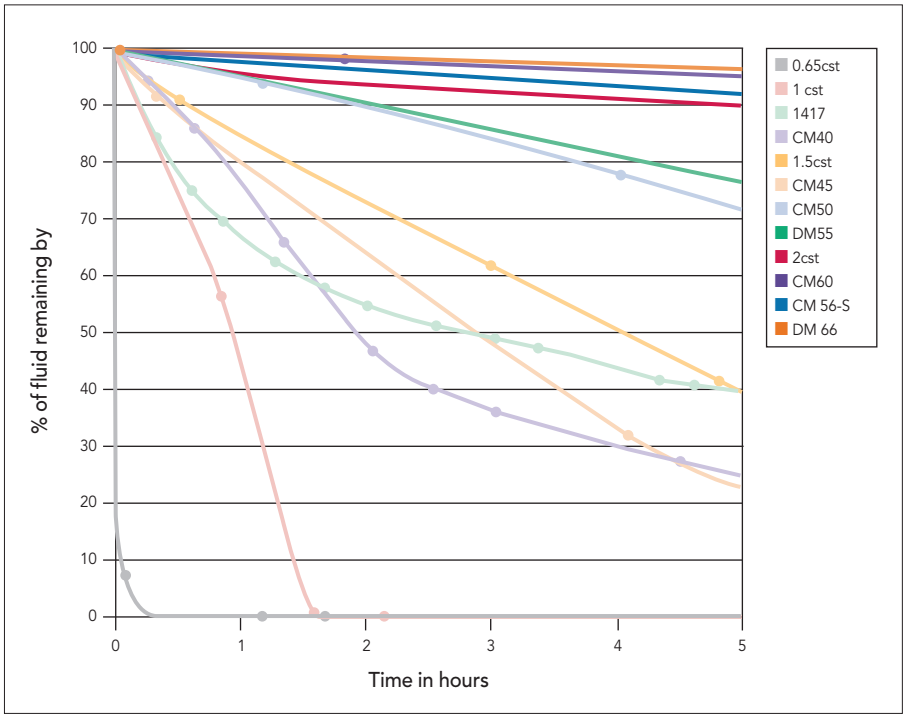

Figure 2: Volatility of BRB silicone fluids at 25°C.

Due to its low heat of evaporation, they deliver no cooling effect during application. Compared to ethanol, they do not dry skin but instead provide a unique luxurious feel.

Volatile dimethicones impart a silky, protective, breathable emollience, and they reduce drying time and tackiness whilst not producing a greasy skin-feel.

Environmental degradability

Nowadays, we are witnessing a high incidence of misconception about silicone's origin and performance. There are significant numbers of blogs and popular press who continue to relate silicone's origin with petroleum derivatives.

In fact, nothing could be further from reality, since silicones come from quartz (sand). Silicon is the world's second most abundant element in the Earth's crust. The chemistry of silicone manufacture involves synthesising, distilling, hydrolysing and polymerising steps to finally obtain

polydimethylsiloxanes (PDMS) which are the bases for producing all the different grades of silicones.

PDMS fluids are insoluble in water. Thus, these silicones when used in rinse-off products transfer to wastewater and become part of the municipal sludge and are very rarely detected in rivers or lakes. Once in the soil, they can degrade by contact with clay components, which will eventually lead to silica and carbon dioxide. Different studies have shown PDMS does not bioaccumulate in living organisms because they are too large to be absorbed by biological membranes.

Concerning low viscosity linear fluids, they may evaporate into the air before entering other environmental compartments such as water or soil. In air, they are degraded in the presence of sunlight, ultimately to silica, water and carbon dioxide.

Table 1: Cross Reference clear odourless emollients for personal care.

INCI	IUPAC	Trade	Short
Cyclotetrasiloxane	Octamethylcyclotetrasiloxane	CM 40, D4	D4
Cyclopentasiloxane	Decamethylcyclopentasiloxane	CM 50, D5	D5
Disiloxane	Hexamethyldisiloxane	DM 0.65	MM
Trisiloxane	Octamethyltrisiloxane	DM 1	MDM
Dimethicone	Decamethyltetrasiloxane	DM 1.5	MD2M
Dimethicone	Dodecamethylpentasiloxane	DM 2	MD3M

Table 2: Properties of volatile siloxanes

Compound	MW (g/mole)	Vapor pressure (mmHg, 25°C)	Solubility (mg/L, 25°C)	Density (g/cm3, 20°C)	Viscosity (cSt, 20°C)	Bp (°K)
D3	222	8.6	1.56	0.856	0.5	408.2
D4	297	0.99	0.56	0.953	2.4	448.7
D5	371	0.174	0.017	0.995	4.2	484.2
D6	445	0.03	0.005	0.966	7.7	518.1
MM	162	42.2	0.93	0.765	0.65	373.6
MDM	236	3.88	0.034	0.82	0.9	425.7
MD2M	384	0.06	7 x 10-5	0.867	1.4	503.1
MD3M	310	0.43	0.006	0.854	1.7	467.1

Non-occlusive agents

One of the principal physico-chemical properties of PDMS fluids is permeability to gas and water vapour. Although silicones are resistant to liquid water, they provide a breathable and non comedogenic barrier when spread over skin.

Several TEWL (transepidermal water loss) tests were run in order to show the no occlusivity and breathable capability of silicones (Table 4).

This test was performed in 10 volunteers and was about to compare TEWL as a function of time between different silicones, a W/Si emulsion and petroleum jelly, known to be occlusive.

After statistical analysis, the result shows there were no significant differences in TEWL between Control, Silicone 1, Silicone 2 and W/Si emulsion with time. Nevertheless, petroleum jelly was the only one to show a significant decrease in TEWL. In fact, petroleum jelly forms a non-breathable layer on skin which minimises the water vapour exchange. Alternatively, silicones and W/Si emulsions do not reduce this epidermal transfer but they permit skin to breathe normally.

As mentioned above, low viscosity dimethicones are synthesised fluids. For this reason, they cannot cause any irritancy or allergy on skin. Despite the fact they are volatiles, they do not dry skin. As we have shown before, they do not reduce transepidermal water loss. Hence, they create a breathable protective barrier skin. For this reason, they are widely used and proposed for sensitive or atopic skins.

Formulations

A bi-phase micellar water (Formulation 1) is a makeup remover lotion with two separate phases. Before using, turn the bottle upside down to apply a homogenous product. After a few minutes, the bi-phase micellar water starts to separate before achieving a clear two-phase product in 1 hour. The bi-phase micellar water (here featuring BRB DM 55) removes face and eye makeup and leaves skin clean and smooth.

Invisible DEO Roll-on is a mild-friendly deodorant specially designed to protect skin, leaving no mark residues on your

Table 3: Solubility profile of low viscosity silicone fluids.

Type of material	Material	BRB DM 0.65 (Disiloxane)	BRB DM 1 (Trisiloxane)	BRB DM 1.5 (Dimethicone)	BRB DM 2 (Dimethicone)	BRB DM 55 (Dimethicone)	BRB DM 66 (Dimethicone)
Highly Polar	Water	I	I	I	I	I	I
Alcohol & glycol	Ethanol	S	PS	PS	PS	I	I
	Glycerin	I	I	I	I	I	I
Sunscreen	Ethylhexyl Methoxycinnamate	S	S	PS	PS	I	I
Hydrocarbon	Mineral oil	S	S	S	S	S	S
	C13-C14 isoparaffin	S	S	S	S	S	S
	Isohexadecane	S	S	S	S	S	S
Vegetable oil	Almond oil	S	S	S	S	I	I
	Castor oil	I	I	I	I	I	I
	Jojoba oil	S	S	S	S	S	PS
	Sunflower oil	S	S	S	S	I	I
Ester	Isopropyl Myristate	S	S	S	S	S	S
	C12-15 Alkyl Benzoate	S	S	S	S	S	S
	Capric/Caprylic Triglycerides	S	S	S	S	S	S
	Decyl Oleate	S	S	S	S	S	S
Silicone	Dimethicone, 350 cSt	S	S	S	S	S	S
	Phenyl Trimethicone	S	S	S	S	S	S
	Cetyl Dimethicone	S	S	S	S	S	S

S=Soluble at all ratio, I=Insoluble at all ratio, PS=Soluble at certian ratio

clothes. It does not contain aluminium salt and is easy to spread, dries quickly and leaves skin soft and smooth. The formulation features: BRB 423: a water in oil emulsifier, BRB DM 55: which provides light emollience, BRB Caprylyl Methicone: which helps spreadability and lubricity, BRB DM 0.65: provides smooth dry skin, BRB SG 516: which gives velvety and powdery feel, and BRB 1736: which offers non-occlusive barrier coat and imparts a silky feel.

Presently, we have been observing significant volume preferences for linear silicones instead of cyclic fluids. Dimethicones BRB DM 55 and BRB DM 66 are precise substitutes to D5 and D5/D6 respectively in terms of viscosity, volatility and sensory.

These replacements can be performed 1:1 and they represent a certain choice to the formulator. Sensory comparison between a deodorant containing BRB CM 50 (cyclopentasiloxane) and its direct linear alternative BRB DM 55 (dimethicone) was performed and shown in Figure 3.

Conclusion

Volatile dimethicones represent an ideal choice to meet both formulators' and consumers 'most exigent current requirements.

Contrary to what the popular press may communicate, volatile linear silicones are not occlusive and protect epidermis with a breathable silky barrier.

As they are inert fluids, they cannot cause any allergy or reaction. Moreover, their high degree of volatility does not dry or affect transepidermal water loss. As a consequence, they are widely used and proposed for sensitive skin.

Table 4: Mean TEWL values ± standard deviation for 10 subjects

Site	TEWL (g/hm²)		
	T0	Tmt	T4h
Control	7.39 ± 1.21	6.80 ± 1.44	6.89 ± 1.37
Silicone 1	7.07 ± 1.19	6.43 ± 1.43	7.15 ± 1.52
Silicone 2	7.38 ± 1.60	6.59 ± 1.95	6.79 ± 1.31
W/Si Emulsion	7.78 ± 1.94	6.36 ± 1.51	6.12 ± 1.49
Petroleum Jelly	8.85 ± 2.53	6.29 ± 2.58	7.56 ± 1.78

Silicone1: BRB DM 1, Trisiloxane. Silicone 2: BRB CM 50. Cyclopentasiloxane

Formulation 1: Bi-phase micellar water (Formula S160514-03)

	Ingredients	INCI	Suppliers	(%)
A1	DI Water	Aqua	Local supplier	49.1
A2	Cophaderm Pentiol natural	Pentylene glycol	Cosphatec	7
A3	Sodium Chloride	Sodium Chloride	Merck	1
A4	Disodium EDTA	Disodium EDTA	Local supplier	0.1
A5	Massocare PEL 64	Poloxamer 184	CQM	2
A6	SunCROMA C39-6393	CI. 42090	Sun Chemical	q.s
B1	BRB DM 55	Dimethicone	BRB	40
C1	Sodium benzoate	Sodium benzoate	Fragon	0.8
Total				100

Low viscosity dimethicones do not bioaccumulate as they are very volatile. They evaporate into the air where they are degraded into silica, H_2O and CO_2. As cosmetic % used and C molecular ratio are quite low, they are not considered as VOC and thus they do not contribute to degrade atmospheric ozone.

Benefits of volatile dimethicones include excellent spreadability, unique non-greasy lubricity, great compatibility with cosmetic ingredients, tackiness reduction and silky, luxurious touch.

They are precise substitutes for cyclics and the new generation of exceptional emollients. PC

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Average results

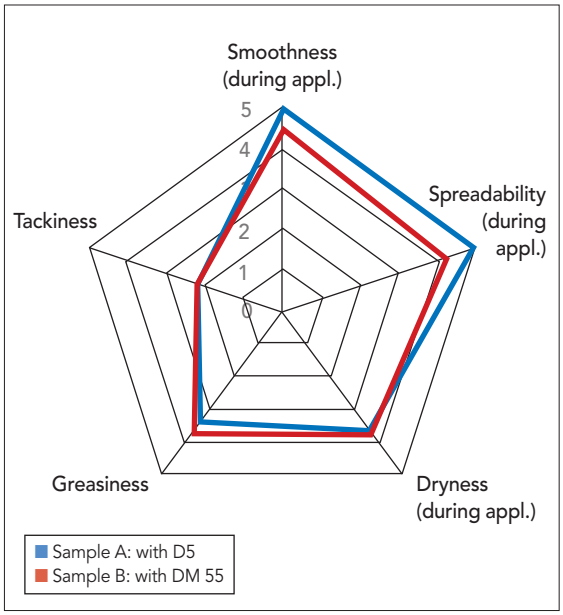

Figure 3: Sensory panel comparing Invisible DEO Roll on with DM 55 versus CM 50.

Formulation 2: Invisible DEO Roll on with DM 55 (Formula S160802-02)

No	Ingredients	INCI	Suppliers	(%)
A1	BRB 423	Cetyl PEG/ PPG-10/ 1 Dimethicone	BRB	2.5
A2	BRB DM 55	Dimethicone	BRB	10
A3	TEC	Triethyl Citrate	Sharon Laboratories	3
A4	Natura-Tec Sunflower Oil Refined	Helianthus Annuus (Sun Flower Seed Oil)	Natura-Tec	2
A5	Microkill COS	Phenoxyethanol, Chlorphenesin, Caprylyl Glycol	Lonza	0.25
A6	BRB Caprylyl Methicone	Caprylyl Methicone	BRB	5
A7	BRB DM 0.65	Disiloxane	BRB	5
A8	BRB SG 516	Dimethicone, Dimethicone/Vinyl Dimethicone Crosspolymer	BRB	1
A9	BRB 1736	Dimethicone and Dimethiconol	BRB	1.5
B1	DI water	Aqua	Local supplier	62.7
B2	Sodium Chloride	Sodium Chloride	Local supplier	1.0
B3	Alcohol	Alcohol	Local supplier	3.0
B4	Butylene glycol	Butylene glycol	Local supplier	3.0
C1	Goldmann Silicone	Parfume	Sillage Aromatique	0.1
Total				100.0