Silicones in Personal Care

Mark Fraser
GE Silicones
April 5, 2004

Agenda
- Introduction to Silicones
- Sand to Specialties - Silicone Chemistry
- Silicone Nomenclature
- GE Silicones product range
- Personal care product forms
- Silicones in personal care
- Silicones in a sunscreen formulation

Introduction

Atomic Symbol: Si
Atomic Number 14
Atomic Weight 28.086
2nd Most Abundant Element
Composed of 28% of Earth’s Crust
Common Form: SiO2, Sand, Quartz, Amethyst

Structure and Characteristics
- Small Change in Physical Properties with Temperature
- Small Change in Physical Properties with Molecular Weight
- Low Tg = 146 K
- Low Modulus
- High Vapor Permeability
Silicone Physical Properties

- Polydimethylsiloxane Backbone Flexibility
  - Easy Orientation at Interface
  - Product Structure Diversity
- Weak Intermolecular Forces, Free Rotation about Si-O Bond
  - Low melting points
  - Low boiling points for lower molecular weight oligomers, D_x, MD_xM, x < 7
  - Small change of viscosity with temperature
  - Low Tg = 146K
  - Liquid at high molecular weights
  - Low Friction with Polymers
  - High Gas Solubility and Permeability
  - High Spreading Coefficient
- Methyl Groups:
  - Low Surface Tension
  - Limited Solubility in Water and Organic Solvents
  - Hydrophobic

Silicone is Unique because of its Chemistry

Periodic Table of the Elements

- Should resemble Carbon Reactivity
- Actually is more like Boron
- Should be Tetra-Valent (but has empty D orbitals)
- Should be Larger than Carbon
- At border between Metals and Non-Metals

Chemistry of Silicone Compounds
Silicon vs. Carbon

\[ \text{Si} - X \quad (X = \text{O, N, Cl}) \]

- Bond is stronger than the carbon analogue
- C-O: 86 Cal/mol Si-O: 108 Cal/Mole C-C: 83 Cal/mol
- Silicon Radius (1.17 Å) is larger than Carbon (0.77 Å)
- C-O: 1.43 Å Si-O: 1.6A
- Silicone is less electronegative than Carbon
  - Bonds to X are more polar
- D orbitals available
**GE Silicones**

**Nomenclature**

<table>
<thead>
<tr>
<th>CH4</th>
<th>Methane</th>
<th>SiH4</th>
<th>Silane</th>
</tr>
</thead>
<tbody>
<tr>
<td>C-OH</td>
<td>Alcohol</td>
<td>Si-OH</td>
<td>Silanol</td>
</tr>
<tr>
<td>C-O-C</td>
<td>Ether</td>
<td>Si-O-Si</td>
<td>Siloxane</td>
</tr>
</tbody>
</table>

- Silanol
- Alkoxy
- Vinyl
- Hydride

**Silicone Shorthand**

- M
- D
- T
- Q

- M*  
- D*  
- T*

**GE Silicones PC Product Family Tree**

- Standard
- Specialty Blends
- Organomodified Silicone and Resin
- Emulsions

- Cyclomethicone
- Dimethicone
- Dimethicone

- SF1173
- SF1204
- SF96-20
- SF1202
- SF96-100

- SF96-5
- SF96-10
- Viscasil 5M
- Viscasil 10M
- Viscasil 12.5M
- Viscasil 30M
- Viscasil 60M
- Viscasil 100M
- Viscasil 50M

- SF96-50

- SS 4230
- SS 4267

- SF 1204
- SF 1214
- SF 1251
**GE Silicones PC Product Family Tree**

**Standard**
- Elastomer
  - SFE 839
  - SFE 818
- Polyether
  - SF 1188A
  - SF 1288
  - SF 1488
- Amino
  - SF 1708
- Phenyl
  - SF 1550
- Alkyl
  - SF 1632
- Resins
  - SF 1318 (Ester)
- SF 1642

**Polymer Network (Resins)**
- Velvesil
- Blend with Cyclomethicone
- Tospearl

**Spherical Particles**
- Polymer Network
- Blend with Cyclomethicone
- Tospearl

**New product**
- SF 1328
- Tospearl 2000B

**Product Forms (technology platform)**
- Lotion/Cream
- Gel
- Solution
- Spray

**GE Silicones PC Product Family Tree**

**Standard**
- Elastomer
  - SFE 839
  - SFE 818
- Polyether
  - SF 1188A
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- Amino
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  - SF 1632
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  - SF 1318 (Ester)
- SF 1642

**Polymer Network (Resins)**
- Velvesil
- Blend with Cyclomethicone
- Tospearl

**Emulsions**
- Amino (Microemulsion)
- Dimethicone
  - SM 2115
  - SM 2125
  - SM 2169
  - SM 2785
- SME 253
- SM 2658

**Organomodified**
- Emulsions

**Blends**
- Silicone and Resin
- Amino (Microemulsion)
- Amino (mini)
- Dimethicone

**Organomodified Emulsions**
- SM 2115
- SM 2125
- SM 2169
- SM 2785
- SME 253
- SM 2658

**Product Forms (technology platform)**
- Lotion/Cream
- Gel
- Solution
- Spray

**Water-in-oil (including silicone) (Mayonnaise)**
- Sunscreen (Neutragena)
- Liq foundation (Lancome, Cover Girl)
- Nivea cold cream
- Generally products with long wearing, durable claims
- Pomades

**Water-in-silicone emulsion**
- Clear Antiperspirant gels (Gillette Series)
- Oil-in-water emulsion
- Eye gel (Pond's)
- Generally Carbomer based

**Anhydrous (grease)**
- Vaseline
- Water-Alcoholic based
- Hand sanitizers
- Fixative (L'Oreal Studio lines)
**GE Silicones**

**Product Forms (technology platform)**

- **Lotion/Cream**
  - Gel
  - Solution
  - Spray

  - One phase, clear dry oil spray (J & J)
  - Capsules (Elizabeth Arden Green tea, Pond’s)
  - Serums (EA Good morning Skin Serum, Lancomb)
  - Astrinrent
  - Facial
  - Clear Shampoo
  - Shower gels

- **Spray**
  - Oil-in-water emulsion
  - Low viscosity (Polo Man’s after shave)
  - Hair detangler spray
  - Solutions
  - Hair spray (alcoholic/water)
  - Suspension
  - Antiperspirant

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**GE Silicones For Personal Care**

Silicones Provide:

- The Dry Feel for Antiperspirants
- The Formulation Vehicle for Clear Gel Antiperspirants and Deodorants
- The Conditioning Agent for 2/1 Shampoos and Hair Conditioners
- A Smooth, Silky, Non-greasy Feel for Skin Care and Cosmetics
- Long Lasting Durability for Color Cosmetics
- Water Resistance for Sunscreens

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**Attributes of Silicones**

**Performance/Functional Benefits**

- Emolliency
  - Lubricity
  - Spreadability
- Uniform film
- Fast Absorption
- Ease of Rub-in
- Play time (color)
- Delivery vehicle
- Emulsifier
- Protection (Hydrophobic)
- Cleansing (solvency, volatiles)

**Sensory Enhancement**

- Soft
- Smooth Feel
- Silky Dry
- Non Greasy
- Non Oily
- Matte (skin and cosmetics)
- Shine (hair, nails, lips)
- Detackification

**Safety Benefits**

- High Thermal and Oxidative Stability
- Non irritating
- Low Toxicity
- Non comedogenic
- Essentially Odorless
**GE Silicones**

### Skin Care Components

- **Emollients:** materials that make the skin feel smoother
  - Organic
  - Silicone (oil free)
- **Humectants:** materials that draw moisture to themselves
  - glycerin
  - silicones generally are not humectants (exceptions are water soluble dimethicone copolysiloxans)
- **Moisturizers:** prevents trans-epidermal water loss (elasticity, smooth)
- **Emulsifiers:** “forces” incompatible ingredients (oil and water) together
  - Dimethicone copolysiloxans (SF1328, SF1528) for water-in-silicone systems
- **Viscosity Control Agents:** thickeners, thinners
- **Specialty Ingredients:** Performance enhancers
  - Durable, long lasting (film formers: SS4230, SS4267)
  - Sensory enhancer, detach (SFE389, SFE818, SF1214)
- **Actives**: Vitamins, antioxidants, sunscreen actives, AHA
- **Fragrance**
- **Preservatives**

### Functional Ingredients

- **Emollient**
  - Light feel
  - Oil-free
  - No-residue
- **Humectants**
- **Moisturizer**
- **Emulsifier**
  - Cyclomethicone and PEG/PPG 2015 Dimethicone
- **Emulsifier**
  - SF1312
  - C30-45 Alkyl Dimethicone
- **Emulsifier**
  - SF1632
  - Ceteary Methicone
- **Emulsifier**
  - SF1642
  - Cyclopentasiloxane and PEG/PPG 20/15 Dimethicone
- **Emulsifier**
  - SF1642
  - Ester modified MQ Resin
- **Emulsifier**
  - SF1555
  - Phenyl Trimethicone
- **Emulsifier**
  - SF1318
  - Phenyl Trimethicone
- **Emulsifier**
  - SF96 series
  - Phenyl Trimethicone
- **Emulsifier**
  - SS4230
  - Bisphenylpropyl Dimethicone
- **Emulsifier**
  - SS4267
  - Bisphenylpropyl Dimethicone

### Clear Water Based Formulate

**Emulsifier**
- Cyclomethicone and PEG/PPG 2015 Dimethicone
- SF1312
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- SF1632
- Ceteary Methicone
- SF1642
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- Bisphenylpropyl Dimethicone
- SS4267
- Bisphenylpropyl Dimethicone

### Opaque Formulate

**Emulsifier**
- Cyclomethicone and PEG/PPG 2015 Dimethicone
- SF1312
- C30-45 Alkyl Dimethicone
- SF1632
- Ceteary Methicone
- SF1642
- Cyclopentasiloxane and PEG/PPG 20/15 Dimethicone
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- SF1318
- Phenyl Trimethicone
- SF96 series
- Phenyl Trimethicone
- SS4230
- Bisphenylpropyl Dimethicone
- SS4267
- Bisphenylpropyl Dimethicone

### Film Former/Transfer

**Emulsifier**
- Cyclomethicone and PEG/PPG 2015 Dimethicone
- SF1312
- C30-45 Alkyl Dimethicone
- SF1632
- Ceteary Methicone
- SF1642
- Cyclopentasiloxane and PEG/PPG 20/15 Dimethicone
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- SS4230
- Bisphenylpropyl Dimethicone
- SS4267
- Bisphenylpropyl Dimethicone

### Hydrophobic/Wash-off Resistance

**Emulsifier**
- Cyclomethicone and PEG/PPG 2015 Dimethicone
- SF1312
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- Bisphenylpropyl Dimethicone
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- Bisphenylpropyl Dimethicone
### GE Silicones

#### Silicons in Skin Care Products

<table>
<thead>
<tr>
<th>Silicone Type</th>
<th>Function</th>
<th>Percentage</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cyclomethicone</td>
<td>Transparent emollient, active carrier, detackify</td>
<td>15%</td>
</tr>
<tr>
<td>Dimethicone</td>
<td>Antisoaping, Ant whitening, emollient, detackify</td>
<td>5.5%</td>
</tr>
<tr>
<td>Cyclcopentasiloxane &amp; Dimethicone Copolyol</td>
<td>Emulsification vehicle</td>
<td>10%</td>
</tr>
<tr>
<td>Gum/fluid blends</td>
<td>Emollient, film former, water repellency, sensory</td>
<td>10%</td>
</tr>
<tr>
<td>Trimethylsilylsilicate</td>
<td>Film former, durability, water-off resistance</td>
<td>5-3%</td>
</tr>
<tr>
<td>Disocystearyl Trimethylpropyl Silox Silicate</td>
<td>Substantive emollient, film former, durability, compatibility with organics, non-migrating</td>
<td>5%</td>
</tr>
<tr>
<td>Alkyl Silicone Waxes</td>
<td>Emollient, moisturizer &quot;silicone petrolatum,&quot; compatible with organics, thickener</td>
<td>1-5%</td>
</tr>
</tbody>
</table>

### Shampoo Components

- **Cleansing Systems**
  - Detergents: Lauryl Sulfates, Laureth Sulfates, Sulfosuccinates, Betains, Sarcosinates
  - Foamer Boosters: Amidoamines, Cocamide MEA, DEA, TEA, Amine Oxides, Polyols

- **Conditioning Systems**
  - Oils: Mineral oil, Dimethicone, Cyclomethicone, Amodimethicone, Lanolin, Fatty Alcohols
  - Cationic Additives: Quats - Triethylmethyl Chloride, Cetrimonium Chloride. Polymers, Amodimethicone, Quaternium-15, -16, Jaguar
  - Viscosity Control Agents
  - Thickeners: Salt, Gums, Cellulose Derivatives, Synthetics, pH Adjusters
  - Thinners: Salt, Alcohol, Glycols, pH Adjusters, “Dimethicone Copolymers”

- **Performance Enhancers**
  - Moisturization (for damaged hair): Dimethiconol emulsions, Amodimethicone
  - Volumizing (for fine hair): Silicone resins, Dimethiconol emulsions
  - Color retention (for color treated hair): Amodimethicone microemulsion
  - Frizz control: dimethicone
  - Fast Drying Time (less damage): Dimethiconol, Amodimethicone

- **Preservative Systems**
  - Additives: Opacifiers, Pearlessing Agents, Fragrances, Colorants
**Hair Fiber Properties Modified by Silicones**

- Frictional: affects combability, feel, body, and hair breakage
- Electrostatic: affects triboelectric charging, or Fly-away
- Visual: affects appearance—luster, gloss, shine, oiliness
- Wettability: affects spreading of water and sebum
- Resistance to Surface Abrasion: affects surface wear
- Interfiber Adhesion: affects hair body and appearance

**Conditioner Attributes**

- Detangle hair after shampooing
- Reduce combing forces for wet and dry hair
- Reduce fly-away
- Improves luster
- Makes hair manageable
- Impart softness
- Adjust pH of hair (after alkaline treatment)
- Temporarily mend split-ends
- Protect hair surface from wear (prevent breakage)
- Reduce drying time

**Water-in-Silicone Emulsification Vehicle**

*INCI*: Cyclopentasiloxane (and) Dimethicone Copolyol

- **Structure flexibility**: x, y, a, b determine Physical
- **Water solubility**: small x, large Y and
- **Organic solubility**: small x, large Y
- **Diverse product probability**

**Emulsifier**
GE Silicones

**Water-in-Silicone Emulsification Vehicle**

**Cyclomethicone (and) Dimethicone Copolyol**

**Cyclopentasiloxane (and) Dimethicone Copolyol**

- Effective in Stabilizing High Internal Phase Emulsions
- Unique Emulsifier allows Excellent Stability at Low Concentrations
  - Emulsifier Lowers interfacial tension
  - Forms boundary barrier, providing stability
  - Smooths out gradient between phases
- Ambient Processing Possible
- Clear Products by Refractive Index Matching
- Excellent Stability
- Non-greasy, Soft feel

**Typical Properties**

**INCI Name:** Cyclopentasiloxane (&) Dimethicone Copolyol

**Solids:** 10-11%

**Diluent/Carrier:** D₅

**Viscosity (25°C):** 20-1,000 cP

**Refractive Index (20°C):** 1.3995-1.4015

* Not intended to be specifications

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**Antiperspirant Gel Formulation**

**Part A**

<table>
<thead>
<tr>
<th>Ingredient</th>
<th>Wt%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cyclopentasiloxane (SF1202)</td>
<td>10</td>
</tr>
<tr>
<td>Cyclopentasiloxane (&amp;) Dimethicone</td>
<td>10</td>
</tr>
<tr>
<td>Copolyol (SF1528)</td>
<td></td>
</tr>
</tbody>
</table>

**Part B**

<table>
<thead>
<tr>
<th>Ingredient</th>
<th>Wt%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rezal 36G (46% salt)</td>
<td>44.5</td>
</tr>
<tr>
<td>DI Water</td>
<td>2.5</td>
</tr>
<tr>
<td>Propylene glycol</td>
<td>25.5</td>
</tr>
<tr>
<td>Ethanol</td>
<td>7.5</td>
</tr>
</tbody>
</table>

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**Multifunctional Silicone Formulation Matrix**

**INCI Name:** Cyclopentasiloxane (&) Dimethicone/Vinyl Dimethicone Crosspolymer

**Japan:** Decamethylcyclopentasiloxane CLSS 520778 (&)Crosslinked Methylpolysiloxane CLSS 523061

**Functions:**

- Emollient
- Sensory Modifier
- Thickener
- Stabilizer
- Delivery System for Actives
- Patented Technology

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**SFE839 Physical Properties**

- **Appearance:** Clear Colorless Gel
- **Silicone Solids (25°C, cP):** 5.25-5.75
- **Worked Viscosity (25°C, cP):** 10,000-30,000
- **Specific Gravity (25°C):** 0.95
- **Density (lb/gal):** 7.98
- **Flash Point (Closed Cup, °C):** 82
- **Freezing Point (°C):** -44

**Silicone Elastomer Dispersion**

- **Cyclopentasiloxane (&) Dimethicone/Vinyl Dimethicone Crosspolymer**
  - Unique Sensory Properties: Dry, Powdery, Lubricious, Cushioning, Easily Absorbed
    - Application emolliency: related to spreading ease
    - Residual emolliency: related to lubricity
  - High Efficiency Thickener for low silicones and esters
  - Stabilizer and Formulation Matrix for Anhydrous Systems
    - No or minimal syneresis
    - Low solid → Minimal interference, better efficacy for active ingredients
  - Cold/Ambient Processing
  - Hydrophobic, Improve Wash-off Resistance and Durability

**Alkyl Modified Silicone Wax**

- **INCI Name:** C30-45 Alkyl Dimethicone
- **Physical Properties:**
  - **Appearance:** Off-white pastille
  - **Melting Point (°C):** 60-70
  - **Density lb/gal (25°C):** 7.35
  - **Compatibility:** Compatible with Organic waxes, Compatible with Silicones
**High RI Fluid Compatibilization**

**Bis-Phenylpropyl Dimethicone: SF1555**

- **Viscosity @ 25°C:** 12 cS
- **Non-irritating**
- **Refractive Index:** 1.46
- **Low Odor**
- **Non Greasy**

**APPLICATION**

- Cuticle Coat
- Spray-on Gloss Products
- Skin Care
- Cosmetics

**BENEFITS**

- Sheen/gloss, compatibility
- Sheen/gloss, compatibility
- Non-greasy, Non-oily, Detackify, Emollient
- Compatible with organic ingredients
- Hydrophobic, Long lasting
- AP/DEO Low residue; raise oil phase refractive index for clear gels

**Bis-Phenylpropyl Dimethicone**

- Specified at 15%
- Meets Oil phase at 11.5%
- SH = Dispersible at 90%
- PSH = Partially Soluble at 1-10%
- SH = Soluble Hot at 10% or higher

**High RI Fluid**

- Water Phase
  - Microfine TiO2 (Hydrophobic)
  - Butylene Glycol
- Oil Phase
  - Cyclododecylsiloxane & Dimethicone Copolyol (SF1528)
  - 8.0 10.0 wt.%
  - Cyclododecylsiloxane (SF1202)
  - 10 16.0

**Sunscreen with SFE839, SF1642 and Physical UV Absorber**

- Oil Phase
  - Dodecyl Neopentanoate
  - 0.5 0.5
  - Isopropyl Myristate
  - 0.5 0.5
  - Butylene Glycol
  - 2.0
  - Water Phase
  - Sodium Chloride
  - 0.2 0.2
  - Water
  - 59.3 61.9
  - Butylene Glycol
  - 2.0
  - Preservative: q.s.

**SF1642 Compatibility**

- **Silicones**
  - Methylbis[(3-Si=O)-ethyl]silane
  - 4,4'-Silylated diphenylsulfone
  - Bisphenol A-xylidene

- **Esters**
  - Hexyl Palmitate
  - 4-Methyl-2-pentanone
  - 1-Octanol

- **Hydrocarbons and Vegetable Oils**
  - Mineral oil 65/75 SUS
  - Petrolatum
  - Castor Oil

- **Waxes**
  - Cetyl Alcohol
  - 1-Octanol

**SF1555 Compatibility**

- **Silicones**
  - Trimethylsiloxydiphenylsilane
  - Triphenylsiloxydiphenylsilane

- **Esters**
  - PEG-8 Diisostearate

- **Hydrocarbons and Vegetable Oils**
  - Mineral oil 65/75 SUS
  - Petrolatum

- **Waxes**
  - Beeswax
## Water-in-Oil Sunscreen with SFE839, SF1555 and SF1642

<table>
<thead>
<tr>
<th>Component</th>
<th>Wt. %</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Oil Phase</strong></td>
<td></td>
</tr>
<tr>
<td>Cyclopentasiloxane (&amp;) Dimethicone Copolyol (SF 1528)</td>
<td>10.0</td>
</tr>
<tr>
<td>Octyl Methoxy Cinnamate</td>
<td>7.5</td>
</tr>
<tr>
<td>Octyl Salicylate</td>
<td>3.0</td>
</tr>
<tr>
<td>Oxybenzone</td>
<td>3.0</td>
</tr>
<tr>
<td>Cyclopentasiloxane (and) Dimethicone/ Vinyldimethicone Crosspolymer (SFE839)</td>
<td>5.0</td>
</tr>
<tr>
<td>Bis-Phenylpropyl Dimethicone (SF1555)</td>
<td>5.0</td>
</tr>
<tr>
<td>C30-45 Alkyl Dimethicone (SF1642)</td>
<td>1.0</td>
</tr>
<tr>
<td>Sorbitan Oleate</td>
<td>0.5</td>
</tr>
<tr>
<td><strong>Water Phase</strong></td>
<td></td>
</tr>
<tr>
<td>NaCl</td>
<td>0.5</td>
</tr>
<tr>
<td>Water</td>
<td>64.5</td>
</tr>
<tr>
<td>Preservative and Fragrance</td>
<td>q.s.</td>
</tr>
</tbody>
</table>

Formulation stability has not been established