TECHNICAL BULLETIN

Zemea® Propanediol: A Natural Solvent for Active Ingredients

Introduction
The relative effectiveness of Zemea® Propanediol as a solvent used to deliver active ingredients and functional materials was modeled and evaluated. The evaluation was conducted using the Formulating for Efficacy software program.

Background
Modern cosmetic skin delivery theory developed by Dr. Johann Wiechers and dubbed Formulating for Efficacy, teaches that step one in building an efficacious formulation is to make sure that a material is well dissolved (through use of a solvent system). The second step is to bring the material to the edge of solubility in a formulation through careful definition of the formulation and the addition of a second ‘driving force’ ingredient.

Water is the universal solvent, but not all materials that a formulator would like to use are soluble in water. Oils can be emulsified, but there are other materials, especially polar molecules, that are only very sparingly soluble in water and need the help of solvents.

Formulating for Efficacy, the Software
The Formulating for Efficacy software is a useful tool that allows formulators to take standard cosmetic ingredients and create formulations that will deliver active materials to the skin. The software program is based on the relationship between formulation composition and skin delivery, and uses Hansen Solubility Parameters (Dispersion [D], Polar [P], and Hydrogen Bonding [H]) to estimate solubility. Each ingredient has a unique set of Hansen values, and materials with similar values will have a high affinity for each other. The extent of the similarity in a given situation, or system, determines the extent of the interaction between each ingredient. The software also calculates the relative difference in polarity for solvent-active and solvent-skin combinations, measured by the Ingredient Active Gap (IAG) and Ingredient Skin Gap (ISG), respectively.

Formulators can quickly find suitable solvents for a particular active material, select ingredient combinations for optimum delivery and design formulations close to the polarity of the skin. For a detailed explanation go to http://www.jwsolutionssoftware.com

Formulating for Efficacy using Zemea® Propanediol
Zemea® Propanediol is a skin-friendly, natural solvent for cosmetics and personal care formulations and has a unique set of Hansen Solubility Parameters. Software modeling suggested that Zemea® can be an effective solvent or driving force ingredient for cosmetic actives and functional materials, when compared to traditional petroleum-based solvents.
Experimental Design

A. Solvents

The following polar solvents (Table 1) were chosen for comparison and are commonly used in cosmetic formulations. The 3-dimensional Hansen space for each solvent (and emollient) relative to the Hansen values for human skin (green dot) is shown in Figure 1. The use of emollients as solvents was not included in this study.

Table 1. Hansen values for common polar solvents

<table>
<thead>
<tr>
<th>INCI Name</th>
<th>δD</th>
<th>δP</th>
<th>δH</th>
<th>MVol</th>
<th>MPl</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aqua</td>
<td>15.5</td>
<td>16</td>
<td>42.3</td>
<td>18.0</td>
<td></td>
</tr>
<tr>
<td>Butylene Glycol</td>
<td>16.1</td>
<td>9.4</td>
<td>24.2</td>
<td>106.3</td>
<td></td>
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<tr>
<td>Glycerin</td>
<td>17.0</td>
<td>12.3</td>
<td>24.2</td>
<td>71.2</td>
<td></td>
</tr>
<tr>
<td>Propanediol (Zemea® natural solvent)</td>
<td>16.8</td>
<td>13.5</td>
<td>23.2</td>
<td>72.8</td>
<td></td>
</tr>
<tr>
<td>Propylene Glycol</td>
<td>16.8</td>
<td>10.4</td>
<td>21.3</td>
<td>73.7</td>
<td></td>
</tr>
<tr>
<td>Dipropylene Glycol</td>
<td>16.0</td>
<td>8.7</td>
<td>21.3</td>
<td>130.3</td>
<td></td>
</tr>
<tr>
<td>Ethanol</td>
<td>15.4</td>
<td>9.2</td>
<td>19.6</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Figure 1. 3D Hansen space of solvents relative to skin

B. Actives

The following active ingredients (Table 2) were chosen for comparison and are commonly used in cosmetic formulations. The 3-dimensional Hansen space for each active relative to the Hansen values for human skin (green dot) is shown in Figure 2. The software program includes active ingredients not included in this study.

Table 2. Hansen values for selected actives

<table>
<thead>
<tr>
<th>INCI Name</th>
<th>δD</th>
<th>δP</th>
<th>δH</th>
<th>MVol</th>
<th>MPl</th>
<th>LogK</th>
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</thead>
<tbody>
<tr>
<td>Allantoin</td>
<td>20.2</td>
<td>24.7</td>
<td>20.2</td>
<td>106.5</td>
<td>230</td>
<td>-3.58</td>
</tr>
<tr>
<td>Ascorbic acid</td>
<td>20</td>
<td>15.7</td>
<td>30</td>
<td>104.2</td>
<td>190</td>
<td>-2.07</td>
</tr>
<tr>
<td>Fenolic acid</td>
<td>19.3</td>
<td>8.4</td>
<td>15.8</td>
<td>155.6</td>
<td>170</td>
<td>1.51</td>
</tr>
<tr>
<td>Salicylic acid</td>
<td>19.7</td>
<td>7.9</td>
<td>15.1</td>
<td>106.6</td>
<td>159</td>
<td>2.18</td>
</tr>
<tr>
<td>Hexylresorcinol</td>
<td>18.2</td>
<td>5.4</td>
<td>11.6</td>
<td>193.5</td>
<td>66</td>
<td>3.67</td>
</tr>
<tr>
<td>Glycolic acid</td>
<td>17.8</td>
<td>12.9</td>
<td>26.9</td>
<td>56.9</td>
<td>75</td>
<td>-0.89</td>
</tr>
</tbody>
</table>

Figure 2. 3D Hansen space of actives relative to skin
Results

A. Maximizing the Solubility of an Active

Example 1. FERULIC ACID – renew and rejuvenate skin texture

Objective: Find a primary solvent to maximize solubility of ferulic acid.

Result: Ferulic acid has high solubility in Zemea®, but not in water.

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Example 2. ALLANTOIN – soothe, stimulate and moisturize skin

Objective: Find a primary solvent to maximize solubility of allantoin.

Result: Allantoin has higher solubility in Zemea® compared to water. Zemea® also works well with Allantoin because it has a relatively smaller difference in polarity compared to the other polar solvents and skin; as measured by the Ingredient Active Gap (IAG) and Ingredient Skin Gap (ISG), respectively.
B. Managing the Solubility of an Active

Example 3. ASCORBIC ACID (Vitamin C) - antioxidant

Objective: Find a secondary solvent to extend delivery time of ascorbic acid.

Result: Ascorbic acid is reasonably soluble in Zemea® and highly soluble in water. Using Zemea® can effectively maximize solubility of ascorbic acid and extend delivery time as the water evaporates from a formulation.

Example 4. GLYCOLIC ACID – exfoliation, anti-aging and skin lightening

Objective: Find a secondary solvent to extend delivery time of glycolic acid.

Result: Glycolic acid has high solubility in Zemea® and water. Zemea® has a lower vapor pressure than water and can extend delivery time as the water evaporates from a formulation while maximizing solubility of glycolic acid.
C. Optimizing a Formulation for an Active

*Example 5. SALICYLIC ACID – treat blemishes and prevent clogged pores*

**Objective:** Optimize a natural formulation of 1% salicylic acid and a fixed 25% oil phase with 2% cetearyl alcohol and 1% caprylyl glycol, using only Zemea® and isostearyl alcohol.

**Result:** Salicylic acid is reasonably soluble in Zemea® and has low solubility in water. The natural formulation can be optimized for maximum delivery using an 11.8% Zemea® propanediol and 9.2% isostearyl alcohol combination.

*Example 6. HEXYLRESORCINOL – lighten and stimulate skin, antioxidant*

**Objective:** Optimize a skin lightening formulation with 1% hexylresorcinol in the aqueous phase of an emulsion.

**Result:** Hexylresorcinol is reasonably soluble in Zemea® and has low solubility in water. The skin lightening formulation can be optimized for maximum solubility and delivery using 17% Zemea® propanediol in a 75% aqueous phase emulsion. Zemea® also works well because it has a low Ingredient Active Gap (IAG) and low Ingredient Skin Gap (ISG).
Conclusion
- Zemea® worked well as a primary solvent to maximize the solubility of ferulic acid and allantoin.
- Zemea® worked well as a secondary solvent to manage the solubility of ascorbic acid and glycolic acid, and extend their delivery time.
- Zemea® worked well as a solvent to optimize the formulation design and efficacy for salicylic acid and hexylresorcinol.

Summary
The relative effectiveness of Zemea® propanediol as a solvent used to deliver active ingredients and functional materials was modeled and evaluated.

The *Formulating for Efficacy* software is a useful tool that allows formulators to take standard cosmetic ingredients and create formulations that will deliver active materials to the skin.

Zemea® propanediol has a unique set of Hansen Solubility Parameters. Software modeling suggested that Zemea® can be an effective solvent for cosmetic actives and functional materials.

Zemea® propanediol is a skin-friendly, natural solvent for cosmetics that provides many performance and aesthetic benefits to skin and hair care formulations.

DuPont Tate & Lyle Bio Products is a joint venture between DuPont, a global science company, and Tate & Lyle, a world-leading renewable food and industrial ingredients company. DuPont Tate & Lyle Bio Products provides natural and renewably sourced ingredients that do not compromise product performance. For more information on the company’s products, visit www.duponttateandlyle.com.

Zemea® is a registered trademark of DuPont Tate & Lyle Bio Products Company, LLC.

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