PREDICTIVE MODELING OF RHEOLOGY MODIFIER FOR LOW pH CLEAR SURFACTANT SYSTEMS

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SUMMARY

The performance profile of the new polymeric rheology modifier, Acrylates Crosspolymer-4 in a commonly used surfactant blend system, Sodium Laureth Sulfate (SLES) and Cocamidopropyl Betaine (CAPB) has been studied via a design of experiments (DOE). Statistical models have been established to predict performance for a given formula or to offer a starting formula to achieve desired performance. A comprehensive understanding of the formulation behavior has been developed. Increasing polymer concentration raises formulation clarity, viscosity and yield value and improves flow texture. Adding more surfactant boosts clarity, viscosity and yield value, but does not necessarily improve flow texture. Raising the level of the secondary surfactant, CAPB at a fixed total surfactant concentration, enhances viscosity and yield value, but reduces formulation clarity and worsens the flow texture.

NEW POLYMERIC RHEOLOGY MODIFIER

Acrylates Crosspolymer-4 is a patent pending emulsion copolymer that has a varying crosslinked gradient zone from the inner core to the surface. This new “hydrodynamic” thicker is designed for formulating high clarity cleansers with unmatched suspension of eye-catching ingredients at low enough pH (4-6) for the use of food grade preservatives.

Figure 1: Schematic Illustration of Swollen Acrylates Crosspolymer-4

Supplied in the protonated form where the polymer molecules are coiled inside the particles. Upon neutralization, the molecules ionize and expand into a three dimensional network due to ionic repulsion.

Figure 2: Benchmark comparison-clarity and bead suspension of different rheology modifiers.

The formula contains 11.2 wt% TS SLES-2, 2.3 wt% TS CAPB with varied rheology modifier usage levels to target sample viscosity at 8,000 mPa.s, at pH 5. Samples were stored at 45°C for 3 months. A: Acrylates Crosspolymer-4 is very clear and keeps bead position unchanged. B: Salt fails bead suspension.

Figure 3: Experimental Design Space

DOE1 confines to 10 wt % TS ≤ “total surfactant concentration” ≤ 23 wt % TS; 1.0 wt % TS ≤ “polymer concentration” ≤ 3.0 wt % TS; 2.25 ≤ “SLES/CAPB blend ratio” ≤ 7. DOE2 restriction condition is that surfactant concentration + 7 x polymer concentration > 22 and surfactant concentration + 2.5 x polymer concentration: 25.

Figure 4: Flow Chart of the DOE Modeling Process.

The test formula contains Sodium Benzoate at pH 5. The Back-Acid Formulating Technique was used.

Table 1: Summary of Performance Corresponding to Increasing the Formulation Factor.

<table>
<thead>
<tr>
<th>Formulation Factors</th>
<th>Clarity</th>
<th>Viscosity</th>
<th>Yield</th>
<th>Texture</th>
</tr>
</thead>
<tbody>
<tr>
<td>Polymer Level</td>
<td>Increase</td>
<td>Increase</td>
<td>Increase</td>
<td>Better</td>
</tr>
<tr>
<td>Surfactant Level</td>
<td>Increase</td>
<td>Increase</td>
<td>Increase</td>
<td>Depends</td>
</tr>
<tr>
<td>SLES/CAPB Level*</td>
<td>Increase</td>
<td>Decrease</td>
<td>Decrease</td>
<td>Better</td>
</tr>
<tr>
<td>CAPB Level*</td>
<td>Decrease</td>
<td>Increase</td>
<td>Increase</td>
<td>Worse</td>
</tr>
</tbody>
</table>

* The factor increases at fixed total surfactant levels.

Figure 5: Correlation between Predicted Results and Experimental Data

The predicted data fit the experimental data very well for viscosity, turbidity and yield. The predicted texture data show the same trend as the experimental data.

Table 2: Predictive Profiler for Formulation Performance.

Formulation performance can be easily predicted by dialing in the potential formula using the profiler. For a specific target performance, a starting formula can be composed by resetting the desirability on the profiler and maximizing desirability according to the targets.

Figure 6: Prediction Profiler for Formulation Performance.

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CONCLUSION

- The DOE provided clear understanding of the relationships between the formulation inputs and their performance.
- Predictive models that fitted experiment data well offered formulation guidance for optimizing performance.
- The most important inputs to achieve target properties were determined.