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Article

Using HSP to Select Coalescents and Improve Film Formation

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TAGS: Science-based Formulation

In dispersion paints, optimal film formation is a crucial factor to achieve coatings with excellent properties and integrity in time. Latex binder systems having a minimum film-formation temperature (MFFT) higher than the temperature at which they will be applied, require the use of a suitable coalescent. By softening the polymer droplets during the crucial period of fusion, it will ensure the film forming process and result in a smooth continuous film[1] upon drying.

Key characteristics of a good coalescing agent are:

- To be an active solvent for the polymer used.
- To lower the minimum film-formation temperature (MFFT) of the polymer.
- To have a lower evaporation rate than water.
- To have a very low solubility in water.

To learn more about coalescing agents, see **Johan Bieleman**'s guide on "Role of Coalescing Agents in Coatings".

Texanol is currently the most widely used coalescent for latex paints in the world: despite sometimes not being the most efficient coalescing aid for a given system, it meets all the above requirements and shows a good cost/benefit ratio.

Still with that in mind, coating formulators may still want to replace Texanol when taking into consideration other properties, such as gloss, hardness development, VOC level, odor, greener profile, etc. And finding alternatives is challenging because they have to meet all the listed requirements.

Good news is that with HSP, you can find an efficient route to replace Texanol in your formulations. *Let's discover how!*

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How Can HSP Identify Good Coalescing Agents?

Dr. Charles Hansen said: *"A good coalescent agent can be identified by plotting the HSP of candidate coalescents with those of the polymer and water in a three-dimensional plot and comparing their respective locations. The good coalescent will occupy the boundary area between the solubility envelope of water and polymer."* [2]

This extra information allows you to **find the right coalescent agent or blend of coalescing agents** for your polymer, in addition to the standard criteria (e.g. high boiling point, low VOC, etc.)

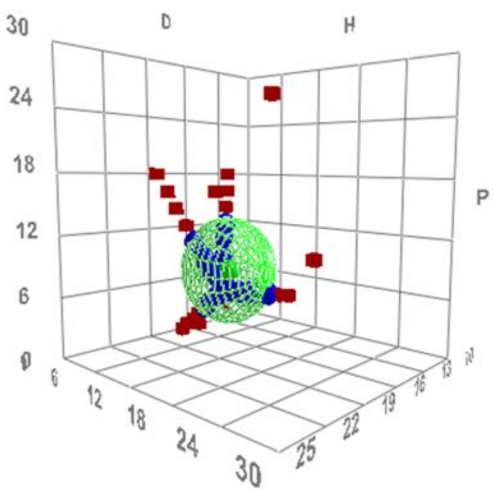
Practically Determining the HSP of a Binder

VLCI practically determined the **HSP of SETAQUA® 6462** by allnex (a styrene acrylic dispersed in demineralized water) as the first step to finding the best coalescing agent possible. This was achieved by adding 0.1 g of SETAQUA® 6462 to 5 mL of various solvents and solvent blends. These were then visually assessed and ranked from 1 – complete compatibility to 6 – complete incompatibility.

When solvents are combined, the HSP of the resulting blend changes to one that lies between the original solvents, in proportion to the amount of each solvent used. By using sets of solvent blends that cross the boundary of SETAQUA® 6462's solubility sphere, it is possible to accurately define the outer limit of the sphere. These rankings were entered into the HSPiP software for analysis.

For more information on the **Hansen Solubility Parameters**, see the articles:

- **Practical Determination and Application of HSP for the Paints & Coatings Industry**
- **Science-based Formulation: The XL Power of HSP for Coatings Compatibility Issues**



Practically Determined HSP of SETAQUA® 6462

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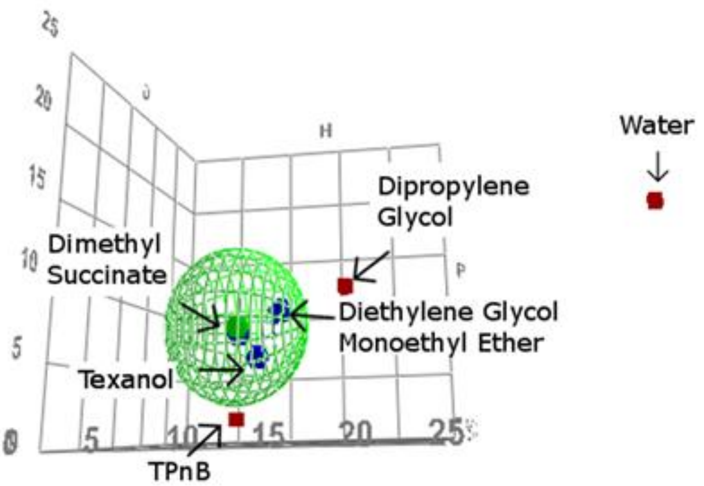
Following Charles Hansen's method, the HSP's of potential coalescing agents were plotted in the 3D solubility space and compared to the HSP of SETAQUA® 6462. From this, we identified some **bad coalescing agents**, which are either too far away from polymer (e.g. **Dipropylene Glycol**) or not positioned appropriately, (e.g. not between the polymer and water, such as TPnB). From these results and using the solvent optimizer in the HSPiP software, **potential good solvent alternatives were selected**.

Due to environmental concerns, the interest in sustainable chemicals is dramatically increasing. In particular, bio-based solvents were analyzed.

Bio-based products are to products wholly or partly derived from biomass, such as plants, trees or animals
(the biomass can have undergone physical, chemical or biological treatment).
– (European Committee for Standardization CEN 2014)

These are shown in the table and image below. They lie in the space between the polymer and water while still being an active solvent for SETAQUA® 6462 (within its solubility sphere). The bio-based solvent selected was Provichem® 2511 Eco **by Proviron**, which is a 100% bio-based solvent, made from **Biosuccinium™ succinic acid**.

Name	Hansen Solubility Parameters			
	δD	δP	δH	Radius
SETAQUA® 6462	16.83	8.07	9.15	5.5
Texanol	15.1	6.1	9.8	–
Provichem® 2511 Eco (Dimethyl Succinate)	16.1	7.7	8.8	–
Dipropylene Glycol	16.5	10.6	17.7	–



3D plot of SETAQUA® 6462, Coalescing Agents and Water

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Validating the HSP Results

A suitable bio-based coalescent has been predicted by the Hansen Solubility Parameters. This was then assessed by a practical test in comparison to the traditional coalescent, Texanol. When a film is made with pure SETAQUA® 6462 a high level of cracking is present, which can be seen in the image below. The two bio-based solvent selected was should improve the film and allow it to form a smooth, transparent, continuous film, while improving other qualities such as gloss.

Surface Defects on a 150 µm Film of Pure SETAQUA® 6462

Blends of 5, 10 and 15% coalescent (on binder solids) with the binder were made and applied to glass panels at a 150 µm film thickness: both coalescents made a smooth, clear film with no surface cracking.

- These panels were then tested after drying, at 48 hours and 4 weeks for gloss evolution and hardness evolution.
- Then the water resistance of the films was tested: a piece of cotton soaked with water was placed on each film.
- To prevent the water from evaporation, a watch glass was placed on top of each cotton piece.
- After 24 hours, the wet cotton pieces were removed, and the films were left to dry.
- The general appearance of the films was evaluated, and the impact on the gloss and hardness was measured.

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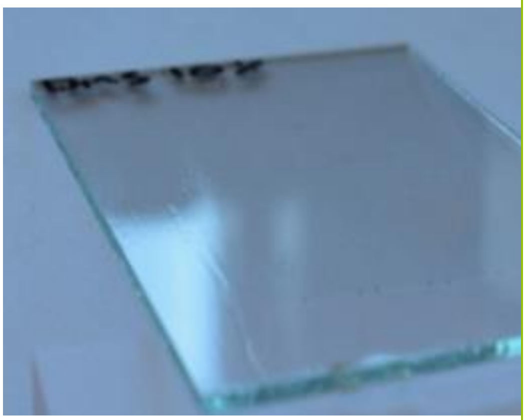
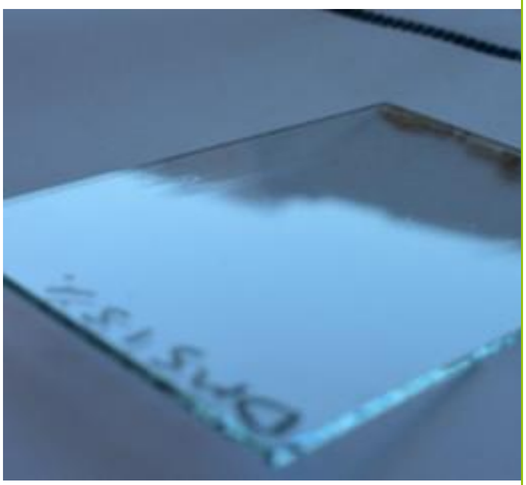
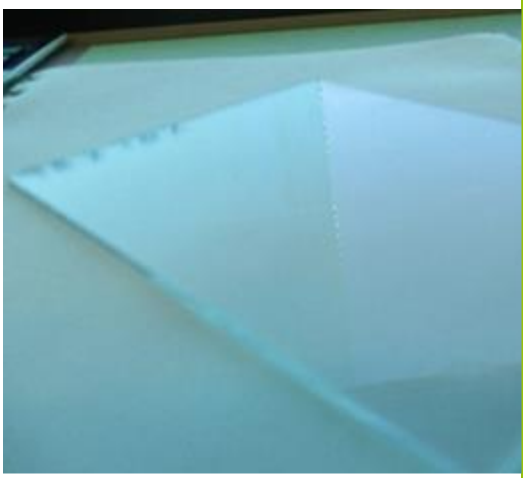
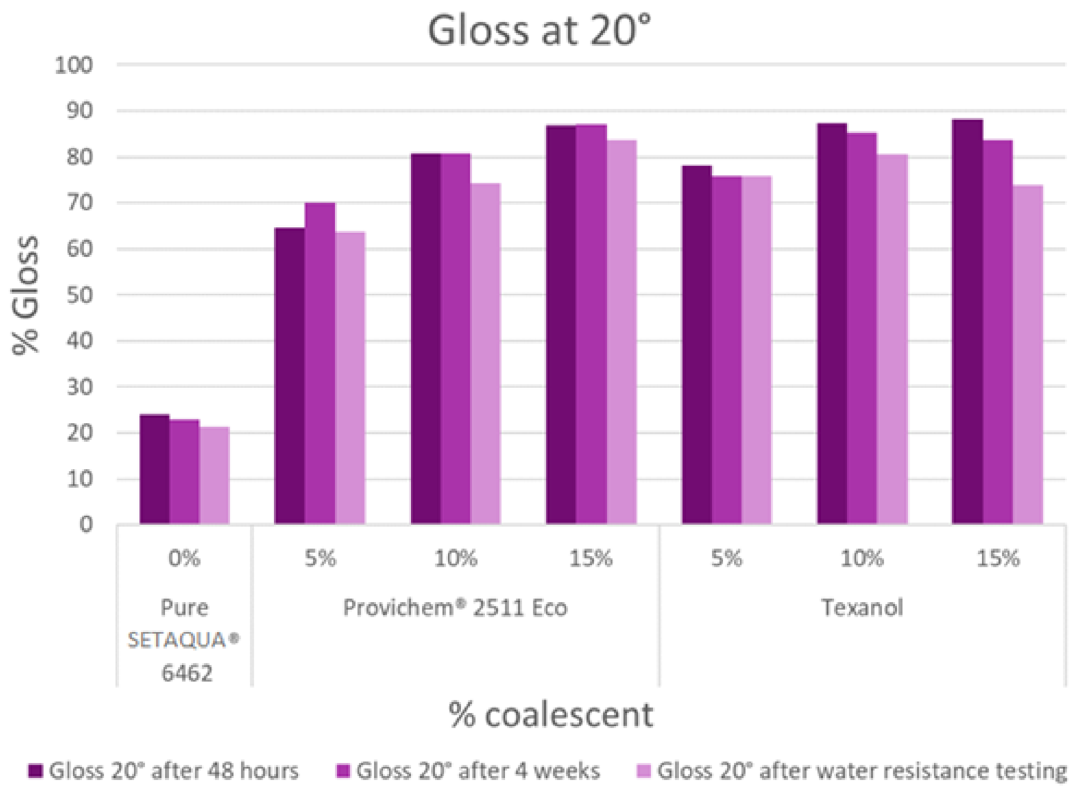
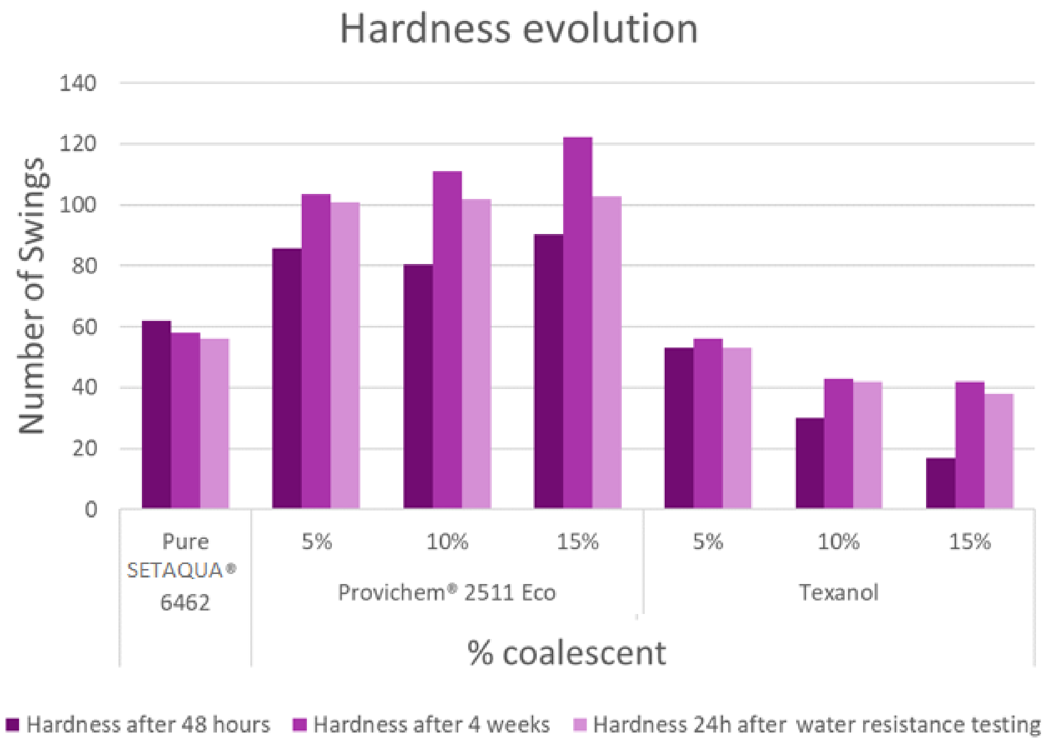
	Appearance of the Films	
	Provichem® 2511 Eco (Dimethyl Succinate)	**Texanol**
5% Coalescent		
10% Coalescent		
15% Coalescent		

Texanol and Provichem® 2511 Eco give a comparable level of gloss at 10 and 15% coalescent. This indicates that both are acting as coalescing agents for the SETAQUA® 6462 and aiding the film formation process.





Provichem® 2511 Eco increases the hardness of the film, whereas Texanol slightly decreases the hardness.

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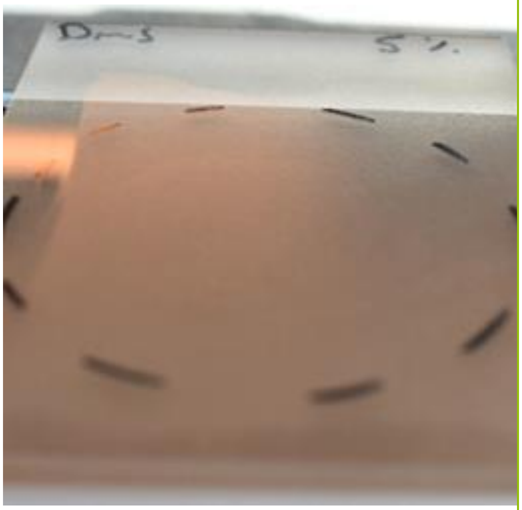
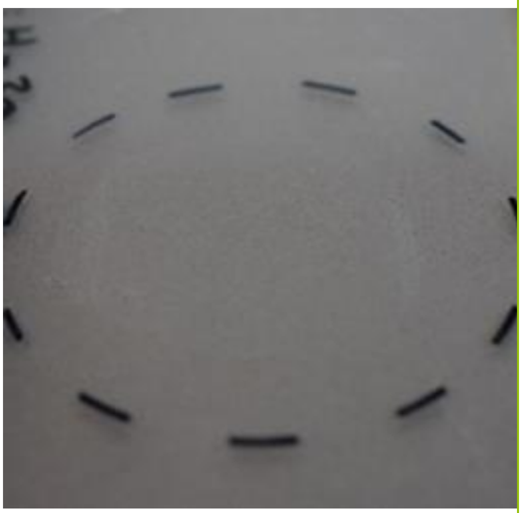
Water Resistance

As seen in the graphs above, all coatings had a slight loss in gloss and hardness after the water-resistance test, but this effect was minor. Aesthetically there were some surface defects after water-resistance testing in the samples with 5% Texanol and 5% Provichem® 2511 Eco, however no visible impact occurred when higher coalescent concentrations were used.

	Appearance After Water-resistance Testing	
	Provichem® 2511 Eco (Dimethyl Succinate)	Texanol
5% Coalescent		
10% Coalescent		

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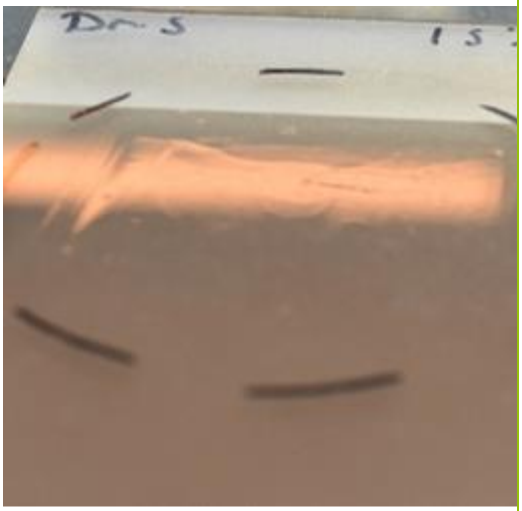
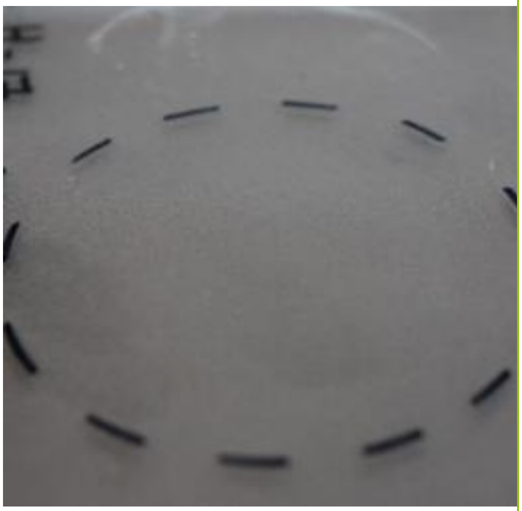
15% Coalescent		

Conclusion

The Hansen Solubility Parameters are a **quick and predictive method** for finding coalescing agents for dispersion paints.

- Provichem® 2511 Eco gave comparable gloss and water resistance with a much higher hardness when compared to Texanol.
- When used in combination with traditional test methods HSP can speed up the raw materials selection or replacement, especially when moving to bio-based or novel materials.

This is just one specific example among many other application possibilities of HSP matching which are worth considering for efficient coating developments. Other typical applications would be:

- [Replacing solvents]
- [Matching optimum dispersants with specific pigments/fillers]
- [Predicting adhesion to a substrate or between layers]
- Enhancing gloss by matching optimum additives or solvents