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Hansen Solubility Parameter System

Solubility parameters are used in the coatings industry to assist in solvent selection. Numerous multicomponent systems have been developed over the years to expand upon Hildebrand and Scott's initial concept of a single solubility parameter. We have found the solubility parameter system developed by Charles Hansen to be especially useful, and it is often referred to in literature describing the properties and performance of DBE solvent.

The Hansen system defines three solubility parameters and relates them to Hildebrand's total or overall parameter by:

$$\delta = (\delta_D^2 + \delta_P^2 + \delta_H^2)^{1/2}$$

where δ_D = Dispersive or "nonpolar" parameter

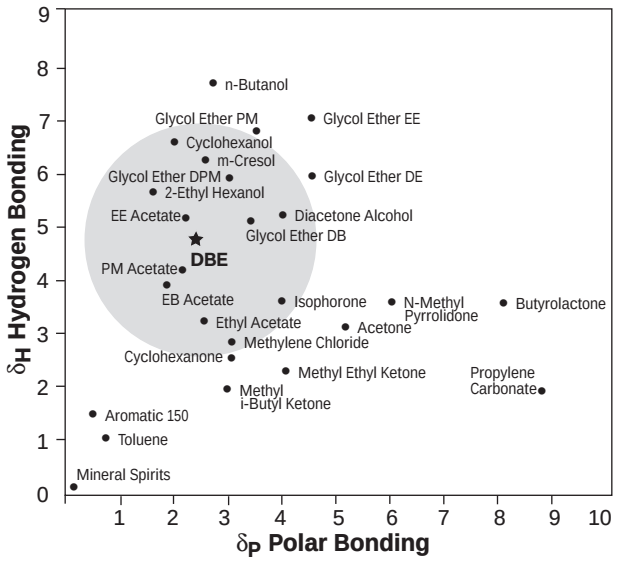
δ_P = Polar parameter

δ_H = Hydrogen bonding parameter

The appropriate values for these component parameters are developed in various ways as discussed in the reference cited. The Hansen solubility parameters may then be plotted in a normal three-dimensional graph. For simplicity, the graphical representation of this "solubility space" is often reduced to a two-dimensional plot of δ_P versus δ_H as shown in **Figure 1**. This is generally an acceptable practice because the dispersive component parameters (δ_D) of many common solvents are quite similar.

Component parameters for polymers may also be assigned and plotted in the same three-dimensional space. The solubility envelope for a polymer may be represented in two-dimensional plots as a circle whose center coincides with the δ_P and δ_H values for that polymer. A coherent volume (or envelope) of solubility is found to exist in this space such that any solvent whose parameters reside within this (envelope) space should dissolve the polymer in question. These plots are referred to as Hansen Solubility Maps. In practice, one can assume that the closer a solvent is to the center of the solubility envelope, the stronger its solvent power for that polymer. Solvents residing outside the envelope are non-solvents for the polymer. The Hansen theory may, therefore, be considered a graphical quantification of the old "like dissolves like" concept of solubility.

Figure 1. Hansen Solvent Map



The real power of the Hansen system for the coatings formulator stems from the fact that a simple mixing rule can be applied according to the following equations to derive the solubility parameters of a solvent blend:

$$\delta_D = \phi_1 \delta_{D1} + \phi_2 \delta_{D2} + \phi_3 \delta_{D3} + \ldots$$

likewise

$$\delta_P = \sum_i \phi_i \delta_{Pi}$$

$$\delta_H = \sum_i \phi_i \delta_{Hi}$$

where ϕ_i = volume fraction of the "i"th solvent in a blend.

The solubility parameters of a blend can be easily calculated (or graphically determined) and a quantitative estimate of the effect of changing solvents or solvent concentration in a blend is quickly obtained. We have found the system very useful when used in conjunction with laboratory experimentation. It is of value not only for its predictive capabilities, but also because it allows for a more systematic approach to solvent formulation.

Figure 1 contains parameter information for DBE and a number of other common solvents. One of the valuable features of DBE solvent is its balance of solubility parameters, which is readily apparent from its centralized location on the Hansen Solubility Map. Solubility parameters of formulations based on DBE may be shifted towards either axis of the map by blending with other solvents providing high performance formulations for a wide variety of coatings resins. More complete solubility parameter data for solvents and polymers may be obtained from the references cited below.

References

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