

## Article

# Practical Determination and Application of HSP for the Paints & Coatings Industry

Sander van Loon – Jun 12, 2018

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The formulation challenges in the paints and coatings industry are miscellaneous and complex. Moreover, “trial and error” continues to be a widely adopted methodology, which is time-consuming, intensive, and increases time-to-market.

**Coating formulations** consist of many different types of raw materials (binders, fillers, pigments, solvents, and additives) which should mix together into one stable and homogeneous dispersion. As the diversity of raw materials available on the market is boundlessly broad, adopting a science-based approach can speed up the development process.



One such approach involves the use of **Hansen Solubility Parameters (HSP)**, which is particularly relevant for predicting ingredients compatibility, and therefore, makes their selection easier for the formulators. This efficiently allows you to narrow down the formulation space as opposed to trial-and-error methods.

In the field of coatings, typical challenges can be tackled by using this approach; for example, HSP can predict an optimal dispersant for a specific pigment/filler (blend), resulting in lower viscosity, as well as lowering the amount of dispersant needed. An **optimal dispersant** will impart maximal hiding power and color intensity, excellent stability against flocculation and will prevent issues such as pigment flooding and floating.

A lower viscosity will be beneficial in many aspects:

- Reduce VOC
- Increase pigment content (in the case of pigment pastes) and solid content in general, and
- **[Extend possibilities for rheology improvements](#)**

In addition, lower amounts of dispersants will raise the barrier performance of the coating and

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can also lead to more cost-efficient formulations. This is just one example among many other application possibilities of HSP which are worth considering for efficient coating developments.

## Smart & Predictive Formulations via Hansen Solubility Parameters

In 1967, **Charles Hansen** submitted his doctoral thesis “**The three-dimensional solubility parameter and solvent diffusion coefficient**” which introduces the theory which has since become known as the Hansen Solubility Parameters (HSP). These parameters have removed the trial-and-error process and given practical solutions to countless problems across a wide variety of formulation-based industries (Hansen, 2017).

The term “**solubility parameters**” is now considered to be quite restrictive, as the use of HSP goes beyond solubility challenges: these parameters can predict the compatibility for various types of chemicals/ingredients, allowing for smart and predictive ingredient matching. Therefore, HSP should be interpreted as “**Hansen Similarity Parameters**”, as recognized by Dr. Hansen.

The Hansen Solubility Parameters are made up of -  $\delta D$  (Dispersion forces);  $\delta P$  (Polar forces) and  $\delta H$  (Hydrogen bond forces). By plotting these in a 3D space in the HSPiP software, it is easy to visualize and interpret the results. When the HSP has been practically determined, the Compatibility Radius is also provided; all solvents/ingredients within this radius are compatible with the test product. The radius is concentration dependent, the higher the concentration of the product the smaller the radius.

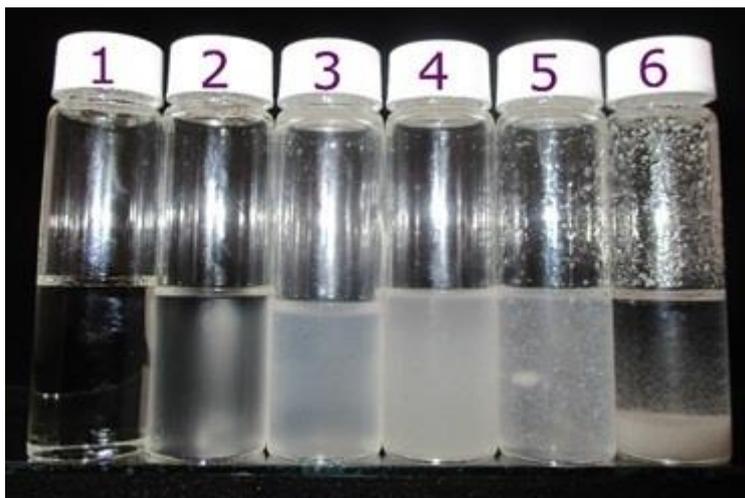
The software HSPiP is now led by Professor Steven Abbott with Dr. Hiroshi Yamamoto. (Abbott, 2017) (Yamamoto, 1999 - Present). VLCI is a certified center for practically determining HSP and has been doing so in close collaboration with **Professor Abbott** and **Dr. Hansen** since 2010, for all areas of the formulation world.

To learn more about the fundamentals of HSP, see Professor Steven Abbott’s Article: [Science-based Formulation: The XL Power of HSP for Coatings Compatibility Issues](#)

## Practically Determining Hansen Solubility Parameters

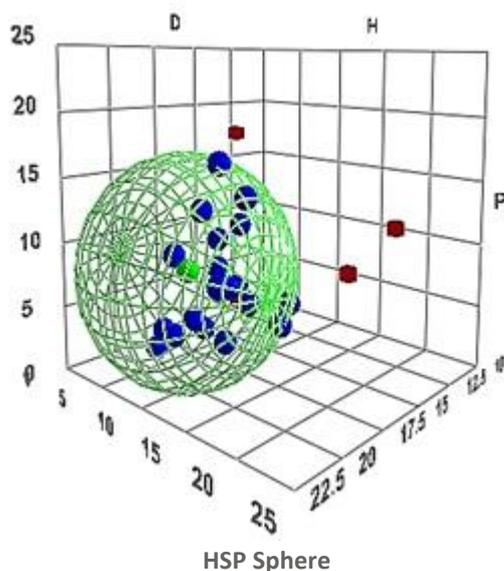
The classic method to practically determine a product’s HSP involves the test material being added to a [range of solvents](#) that cover the HSP space. The samples are shaken and left to dissolve. The samples are then visually assessed with a qualitative rank from 1-6, where a 1 means the product is completely dissolved, a 6 means there has been no interaction between the solvent and the product and the other scores indicating various stages of dissolution.

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Stages of Dissolution

This data is then entered into the HSPiP Software, which defines a spheroidal cluster of the solvents that dissolve the test material. This cluster is called the Hansen Solubility Sphere and its central coordinates ( $\delta D$ ,  $\delta P$  and  $\delta H$ ) define the solubility parameters of the test material. The software also performs an analysis of the “fit” of the data to the parameters it has determined, highlighting the validity of the result, which can indicate if more experimental data is needed.



This theory can be applied to a wide range of situations, including crosslinked (insoluble) polymers, [additives](#), [pigments](#), nanoparticles etc. The scoring is then based on criteria such as swellability or resistance to sedimentation, VLCI offers the following test methods and HSP workflows for a range of materials and is able to develop bespoke tests for challenging molecules:

Method	Suitable for
Dissolution Method	Simple solutes, mixtures, additives
Quantitative Swell Test	Crosslinked and insoluble polymers
Sedimentation Method	Insoluble particles, e.g. pigments
Liquids Method	Low molar volume liquids, e.g. solvents

Polymers, surfactants, solvents, insoluble pigments, films, complete formulations and much more can be practically determined!

## Interpreting the Results

The HSP parameters of a raw material give lots of information, but there are many useful ways to implement and interpret them. The HSPiP Software defines the Relative Energy Difference (RED) of any product (solvent, polymer, particle...) to the test material; this is calculated by these two equations:

$$\text{Equation 1: } R\alpha^2 = 4(\delta D_1 - \delta D_2)^2 + (\delta P_1 - \delta P_2)^2 + (\delta H_1 - \delta H_2)^2$$

$$\text{Equation 2: } RED = R\alpha/R_o$$

$R_o$  is the radius of the material's compatibility sphere. The RED value is very useful when formulating and can be interpreted by the following definitions:

- RED = 0 the product and material have the same HSP.
- RED < 1 the product lies within the materials' compatibility sphere and therefore will be compatible.
- RED = 1 the product lies at the boundary of the material's compatibility sphere, so will be borderline compatible. Hansen has noted that many smart formulations work at the borders!
- RED > 1 the product lies outside the material's solubility sphere and therefore is incompatible.

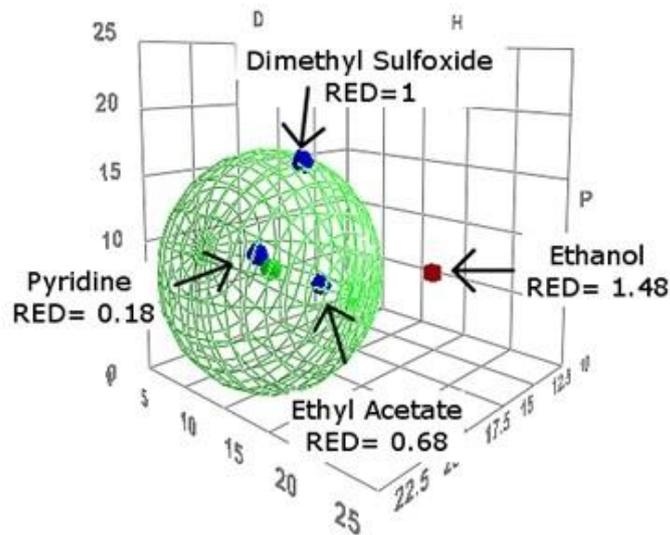
These rules apply to issues, such as:

- Dissolving polymers
- Finding compatible plasticizers
- Promoting adhesion between inks and polymers
- Identifying polymer/nanoparticle combinations, and much more

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In principle, materials with the lowest RED are the most compatible to each other, selecting these will allow you to formulate at the lowest concentration, and will give the maximum performance in the formulation.

For example, if a pigment/filler and dispersant have a RED close to 0, the minimum amount of dispersant will be needed to stabilize the pigment/filler and will reduce the viscosity the most.



Examples of Relative Energy Differences

When searching for new raw materials, the RED values, or just the rankings of Ra (“distance”) values, are crucial for predicting the compatibility between formulation ingredients and therefore allowing you to choose materials that are more likely to be right first time.

By learning more about the nature and compatibility of ingredients with HSP, it is possible to formulate with the minimum concentration, while achieving utmost performance. Applying HSP in this way allows the selection of suitable ingredients with certain properties in an efficient and effective manner.

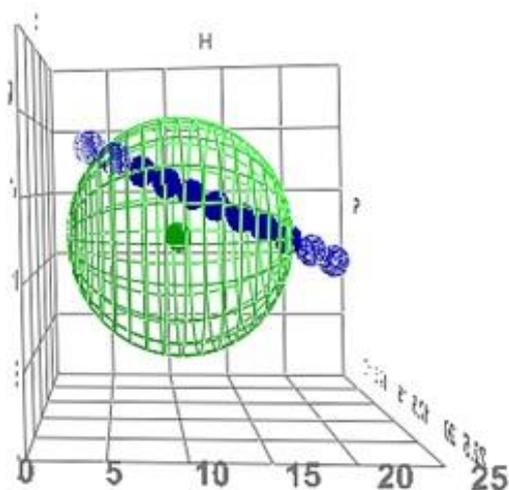
## Implementing Hansen Solubility Parameters

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. This is shown in the image below, where Propylene Carbonate and Propylene Glycol are blended in steps of 10% (e.g. 90:10, 80:20, 70:30...).

In this example, both Propylene Carbonate and Propylene Glycol lie outside of the solubility sphere and therefore are “**bad solvents**”. Upon blending these solvents, certain combinations become “**good solvents**” and will dissolve the material. This is an extremely useful application of HSP which can swiftly create novel solutions to problems that otherwise could cause major delays to projects.

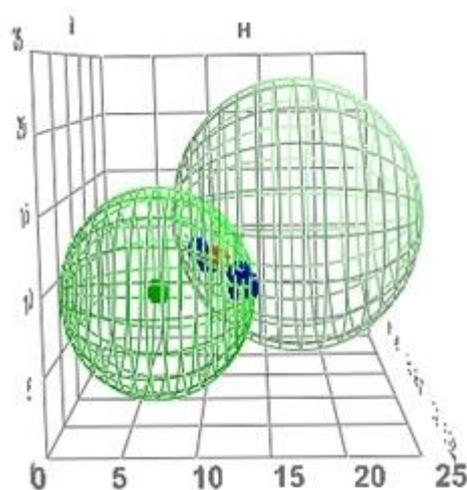
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It allows the formulator to think outside the box (or the sphere!), taking a component that is desirable for other reasons (e.g. low cost) and rationally matching it with another component to create a high-performance solution.



**Examples of the HSP of Solvent Blends between Propylene Carbonate and Propylene Glycol**

If two or more raw materials are incompatible, by determining the HSP spheres of all materials, you can then see if there is any region of overlap of their spheres. Products that lie within the overlap of the solubility sphere of all materials will aid the overall compatibility of the system. If there is no overlap between the ingredients, it is still possible to find an ingredient that lies between the two in the solubility space. This third ingredient can bridge the gap between them and again aid the overall compatibility.



**Examples of Finding Solvents within the Overlap of 2 Incompatible Products Solubility Sphere to aid Compatibility**

## Theoretical Predicted or Practically Determined?

HSP parameters of most molecules can be theoretically predicted from their **SMILES**, by using the Yamamoto-Molecular Break (Y-MB) which breaks SMILES into the corresponding functional groups and estimate's their various properties. The predictive power of the software is an impressive achievement, yet is not perfect and contains known errors.

HSP theory was originally developed to be a practical test and by practically determining the HSP of molecules or products you can be confident that this theoretical error is removed and that you have true HSP values of your product. It is only possible to theoretically predict the D, P and H values and not the Solubility Radius, which is a vital piece of information for many aspects of formulating and to truly implement the HSP of your product. By practically determining the HSP of your product the Solubility Radius will be calculated, which can even be tailored to the specific concentration of your final formulation.

If you wish to discuss the possibility of determining the HSP of a product, please contact SBF.G.

### About the Co-Author

**Beverley Fricker** is a Formulation Chemist and Hansen Solubility Parameters expert at VLCI (Van Loon Chemical Innovations), an independent laboratory providing innovative and practical R&D services within the formulation industry. With the unique approach of combining applied formulation science with High Throughput (HT) screening, VLCI aims to move the formulation industry to a higher level, creating flexibility, predictability, new insights/products and efficiency.



After gaining her BSc in Chemistry from the University of Sheffield, she worked in research on formulation and product development at AkzoNobel (coatings), then at RB (personal care and household products). Currently at VLCI, she specializes in determining Hansen Solubility Parameters and implementing them into the overall formulation process across the entire formulation industry.

### References

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