https://polymer-additives.specialchem.com/tech-library/article/flavor-scalping-of-a-biobased-polymer-predicted-by-hsp

Article

Flavor Scalping of a Bio-based Polymer Predicted by HSP

Sander van Loon – Dec 13, 2018

TAGS: **Science-based Formulation** **Bio-based Solutions**

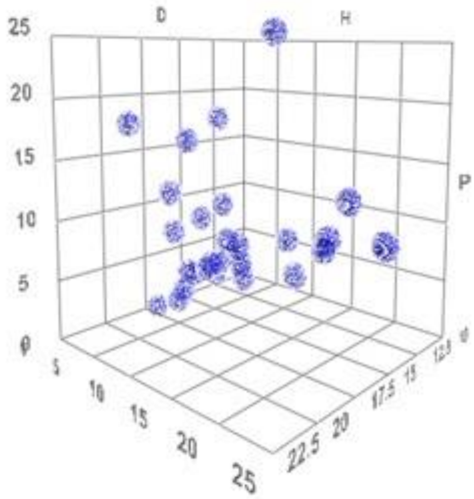
Packing continues to be one of the biggest markets for plastics. But, there are growing environmental concerns due to the origin of petrochemicals and long life-cycles of plastics.

Though recycling has become much more widespread, roadblocks still remain. This has caused the industry & the scientific community to search for alternatives. One such route is via **bio-based polymers**.

The European Standard EN 16575:2014 '**Bio-based products – Vocabulary**' defines the term bio-based product refers to products *wholly or partly derived from biomass*, such as plants, trees or animals (the biomass can have undergone physical, chemical or biological treatment). The key to successful implementation of bio-based polymers to replace traditional polymers is to know as much as possible about the material before starting processing.

To do this quickly, instead of trial-and-error testing, you can use Hansen Solubility Parameters (HSP). With HSP, you can quickly:

- Characterize new materials
- Predict practical solutions for the solubility and compatibility of new materials



Hansen Solubility Space

https://polymer-additives.specialchem.com/tech-library/article/flavor-scalping-of-a-biobased-polymer-predicted-by-hsp

To understand how to apply this in practice, let's take 2 such bio-based polymers, which help address the environmental concerns in two different ways.

1. Bio-polybutylene succinate, and
2. Bio-polybutylene succinate adipate

Bio-PBS and Bio-PBSA are bio-based polymers from PTTMC. PTTMC is a strategic joint venture between PTT Global Chemical Public Company Limited (PTTGC) and Mitsubishi Chemical Corporation (MCC).

Bio-PBS and Bio-PBSA are food contact grade crystalline polyesters which are produced from Succinic Acid and 1.4-Butanediol (BDO). Bio-PBS is naturally compostable at 30°C to H2O, CO2 and biomass without composting facility.

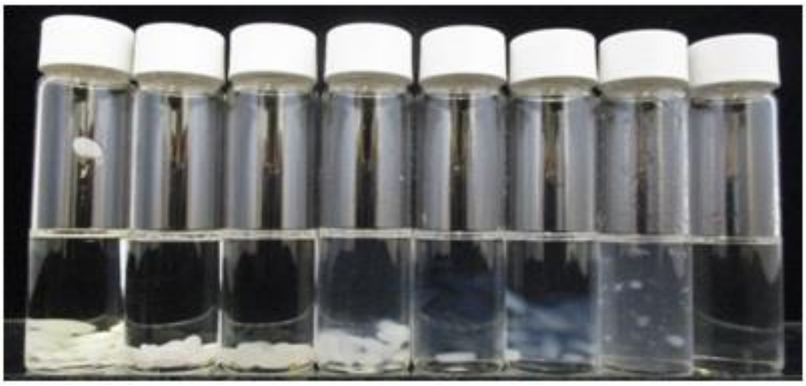
The Succinic Acid used is from Succinity® which is a joint venture between BASF and Corbion. They use a proprietary production process in which bacteria or yeasts in a bio-reactor (fermenter) transform biomass, starch or sugar into the desired acid.

Practically Determining the HSP of a Bio-based Polymer

VLCI practically determined the HSP of Bio-PBS and Bio-PBSA. This was achieved by adding 0.25 g of the polymer to 5 mL of **various solvents** and solvent blends. The samples are shaken and left to dissolve. The samples are then visually assessed with a qualitative rank from 1 to 6, where:

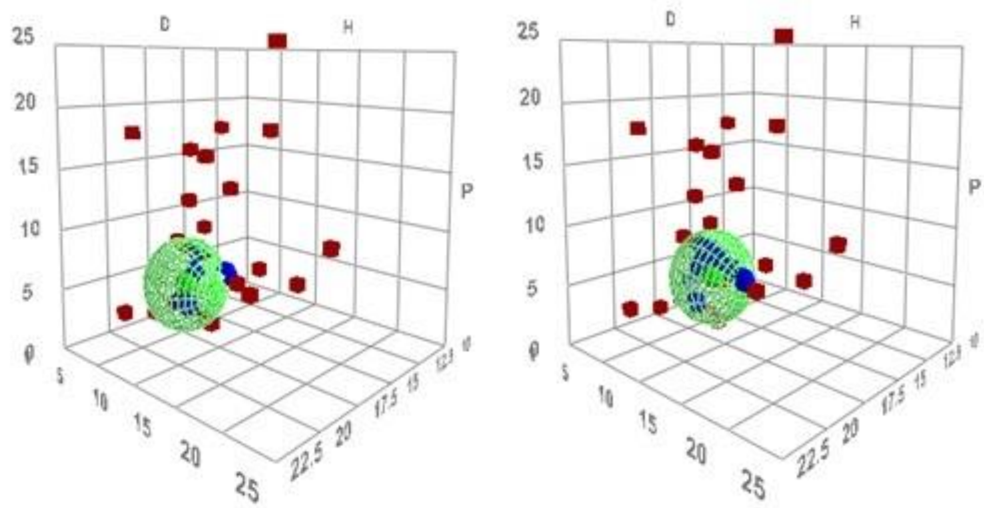
- 1 means the product is completely dissolved,
- 6 means there has been no interaction between the solvent and the product, and
- Other scores indicating various stages of dissolution

https://polymer-additives.specialchem.com/tech-library/article/flavor-scalping-of-a-biobased-polymer-predicted-by-hsp



The Visual Differences Seen in the Samples

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 the polymers solubility sphere, it is possible to accurately define the outer limit of the sphere.



Defining Outer Limit of Bio-based Polymers HSP Sphere

For more information on the Hansen solubility parameters, see the article:
Calculating 'Like' and 'Unlike' using HSP in Plastic Formulations

This ranking data is then entered into the HSPiP Software, which defines a spheroidal cluster of the solvents that dissolved the test material. This cluster is called the Hansen Solubility Sphere and its central coordinates (δD, δP and δH) define the core 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.

https://polymer-additives.specialchem.com/tech-library/article/flavor-scalping-of-a-biobased-polymer-predicted-by-hsp

Product Name	D	P	H	R	Fit
Polybutylene Succinate	18.63	5.55	7.99	3.8	1.000
Polybutylene Succinate Adipate	17.67	5.34	7.19	2.7	0.930

With the HSP of polymers, it is then possible to predict compatible **plasticizers**, co-solvents and various other molecules to aid the processing of the polymer. Also, the stability of the polymer and the product contained within it can be predicted.

Addressing the Flavor Scalping Issue with Hansen Solubility Parameters

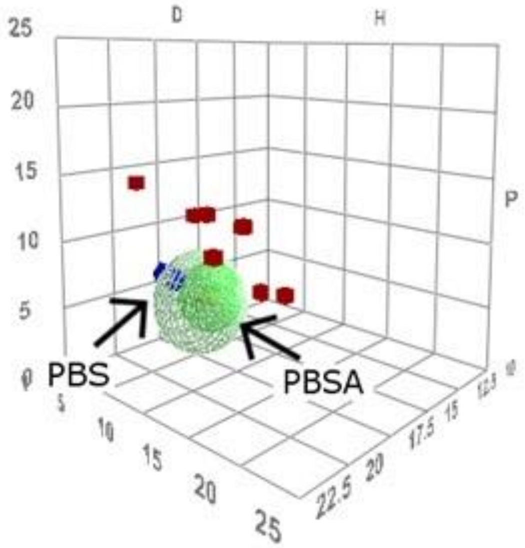
Sorption of flavor and fragrance compounds by plastic packaging materials is a major factor contributing to the quality degradation of foods and other products during storage. This causes changes in both the intensity and characteristics of the products flavors/fragrances. This is because of their absorption by the packaging material, a phenomenon commonly referred to as "scalping".

It has been shown many times that scalping can be predicted by comparing the HSP of polymer to the HSP aroma compounds. The distance at which a flavor will have an affinity for a polymer is specific to each pairing; however, a general rule is a distance of 8 units.

Below is a comparison of common flavor compounds and the 2 bio-polymers (PBS and PBSA).

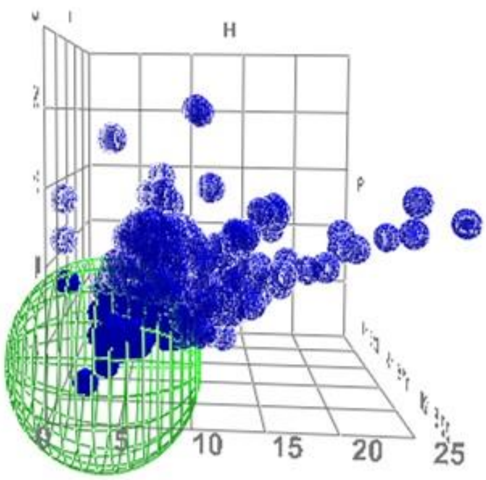
Flavour	Compound	Distance to PBS	Distance to PBSA
Cinnamon	Cinnamaldehyde	2.82	3.06
Almond	Benzaldehyde	3.61	4.45
Gravy	3-mercapto-2-methylpentan-1-ol	5.04	4.76
Vanilla	Vanillin	5.54	6.92
Chilli	Capsaicin	6.56	6.84
Olive	1-Hexanol	7.09	6.40
Straw	4-hydroxy-2,5-dimethylfuran-3-one	7.59	8.27

Beer	Isovaleraldehyde	9.29	7.58
Bread	Maltol	11.29	12.06
Nutty	2-Acetylthiazole	11.27	11.08

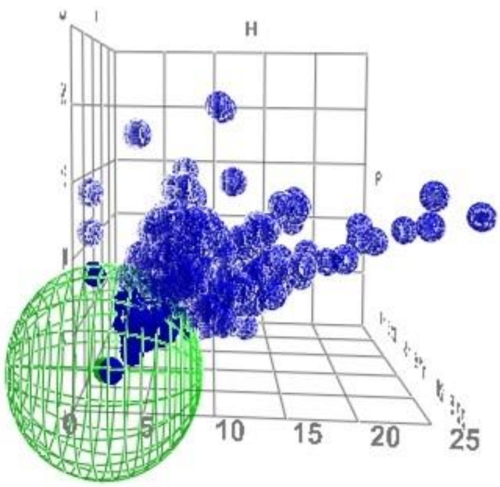


From this data, before any stability testing takes place, it is observed that cinnamon flavored products are predicted to be too compatible with the product and therefore not suitable for packaging in BioPBS. Whereas, nutty-flavored products are predicted to be fine (incompatible). This can drastically speed up screening for **packaging material selection**.

In comparison to the more traditional polymers below, Polyethylene and Polypropylene, we can see that PBS and PBSA have a much smaller solubility sphere. So, they are overall are more chemically resistant polymers.



Polyethylene



Polypropylene

https://polymer-additives.specialchem.com/tech-library/article/flavor-scalping-of-a-biobased-polymer-predicted-by-hsp

Conclusion

Hansen Solubility Parameters are a very powerful tool when it comes to working with novel, uncharacterized materials and when selecting packaging for final products. It can help to select compatible chemicals for the processing of polymers or to:

- Find **greener, safer alternatives** for existing processing chemicals, as well as
- Predict the stability issues of packaging with final products

Practically determining the HSP polymers is a very quick method to understand the materials you are working with and offers many different ways to implement the data.

References

1. Adrien Benazzouz, Laurianne Moity, Christel Pierlot, Michelle Sergent, Valérie Molinier and Jean-Marie Aubry. 2013. “Selection of a Greener Set of Solvents Evenly Spread in the Hansen Space by Space-Filling Design.” *Ind. Eng. Chem. Res*. 52: 16585-16597.
2. Denis Prat, Andy Wells, John Hayler, Helen Sneddon, C. Robert McElroy, Abou-Shehadad and Peter J. Dunne. 2016. “CHEM21 selection guide of classical- and less.” *Green Chemistry* 18: 228.
3. European Committee for Standardization CEN. 2014. “EN 16575:2014 ‘Bio-based products – Vocabulary’.”
   (Roland and Hotchkiss 1991)
4. https://www.hansen-solubility.com/HSP-examples/flavor-scalping.php