Development Parameters for High Performance Dispersing Agents for Industrial Coating Applications.

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Introduction

Dispersants are a key component of industrial coatings and inks. Although often, their content in the formula is low in comparison with other components such as pigments, fillers or solvents, their function is crucial, as they allow for high solids loading dispersions with low viscosity, and also ensure dispersion stability by preventing the solid particles agglomerating and settling. This way, formulators can develop high solids coatings and inks that are stable for long time and produce bright and uniform colours with no spots or defects.

The molecules that enable the above performance are complex polymeric structures that combine one or more types of functional groups with chemical affinity for the solid surface, (the anchor groups), with polymeric chains of variable length with affinity for the liquid phase that can extend through the solvent, providing stability against flocculation and settling, (the stabilisation chains.)

In this paper, we will review the target requirements of a dispersing agent, intended for stabilization of high loading very fine solid particulate, that we will call hyper-dispersants. The function and structure of anchor groups and stabilization chains will be analyzed to show design process of a dispersant molecule.

Hyper-dispersants, definition and requirements

We could define a hyper-dispersant as a molecule designed to allow solids particulate, of very high surface area, to be evenly distributed in a continuous (liquid) phase becoming a stable fluid with no phase separation or settling issues.

In a way, the hyper-dispersant acts as an interphase between the solid particles and the liquid phase, making them compatible, so that the particles dispersed in the liquid make a system energetically stable.

To achieve the performance described, the main technical requirements of a hyper-dispersant would be:

- Capable to produce low viscosity-high solids dispersions
- High colour development
- Good stability
- Broad pigment compatibility
- Broad resin compatibility

And, taking into account other boundaries such as market demands, regulatory constraints or even the production process characteristics, the likes-to-have would be:

- 100% active product
- Pourable liquid form
- Sustainable content
- Broad regulatory clearance
- Low hazard rating
- Low cost

Morphology of a hyper-dispersant and its function through the milling process

A milling process is typically described as a particle reduction process by mechanical means that takes place in three differentiated phases:

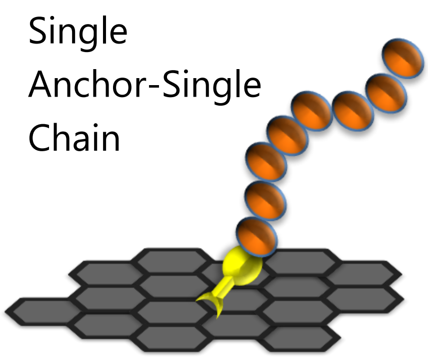
1. The first step is the wetting phase, in which a surfactant or wetting agent can assist.
2. The second step is the grinding part. It is a mechanical attrition step in which the dispersant plays no part
3. The last step is the stabilizing phase where the dispersant is essential to reach the desired performance

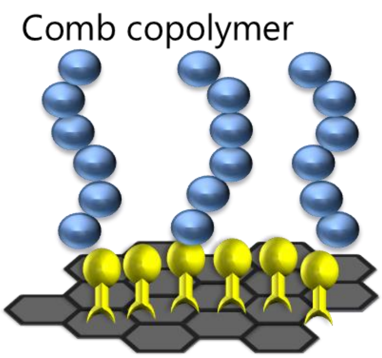
There are two different stabilizing mechanisms:

- **Electrostatic stabilisation:** charged polymers adsorbed on the surface of the particles act like small magnets and repel, thus keeping particles apart.
- **Steric stabilisation:** the head of the polymer adsorbs to the particle surface and the chain projects into the media. This creates an area of high osmotic pressure around the particle, causing repulsion.

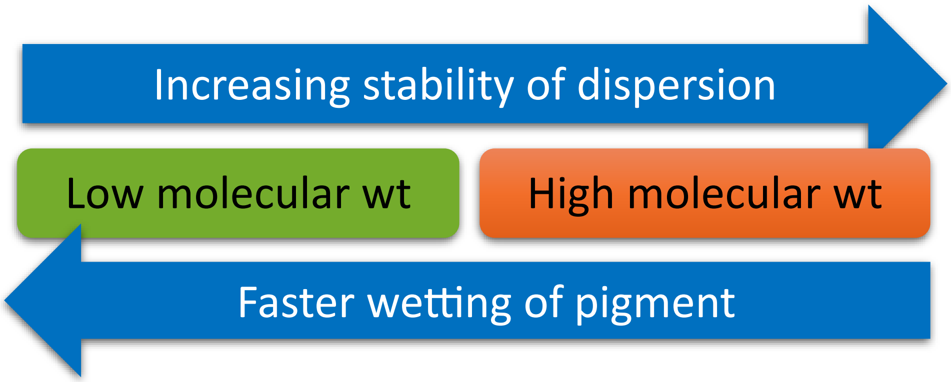
With the above in mind, the most usual molecule structures of a hyper-dispersant are:

- Polymer with terminal functional groups (single anchor/single chain)
- Polymer with functional groups at each end
- BAB Block copolymer
- ABA Block copolymer
- Random copolymer
- Comb copolymer





These differentiated morphologies determine important characteristics of a dispersant, such as the molecular weight which, in turn, determines its wetting or stabilizing character, as seen in the chart below:



For this reason, the preferred structure for hyper-dispersants is usually the comb structure, i.e. the one of higher molecular weight, because in industrial applications, often, stability is more important than fast wetting.

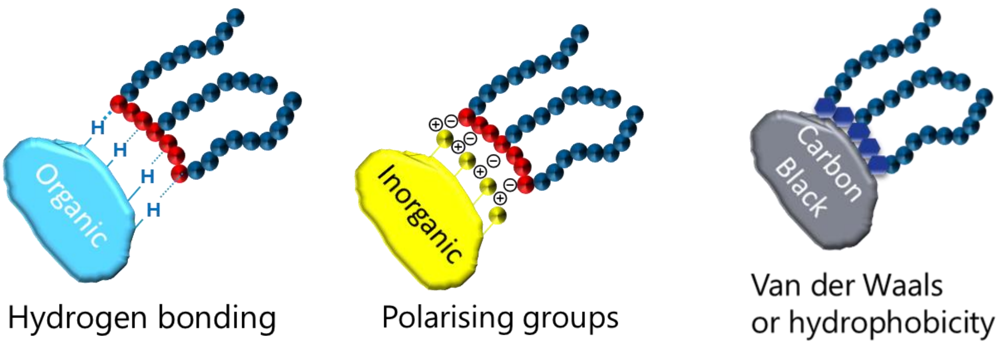
Functional groups of a hyper-dispersant. Key features and properties

Let's have a look at the main characteristics of each one of the two differentiated parts of a hyper-dispersant, the anchor group and the solubilizing chains, as both anchor and stabilising polymers influence the physical form of the product.

<u>The anchor group</u>

The anchor group must attach to the pigment surface strongly. So, different pigment surfaces will require different anchor groups. In other words, different chemical characteristics of the pigment surface, will dictate the chemical nature of the anchor group, as the anchoring mechanism will be different. So, we find that:

- Organic pigments. The predominant anchor mechanism is hydrogen bonding
- Inorganic pigments. The predominant anchor mechanism is ionic bonding
- Carbon black. The main anchor mechanism are Van Der Waals forces or hydrophobicity.



The anchor polymer dictates which pigments it will be effective with- but also has an influence on product cost.

The most common chemical species used in dispersants with multiple anchor points are:

- Polyamine
- Polyurethane backbones
  - acid or amine functional
- Quaternized amine
- Polyaromatic
- Mixed polyaromatic / amine
- Functionalized acrylics

The stabilizing chains

The steric stabilizing chain must be the correct length. If too short it will not overcome the attractive forces whereas, if too long, it could fold back and become entangled.

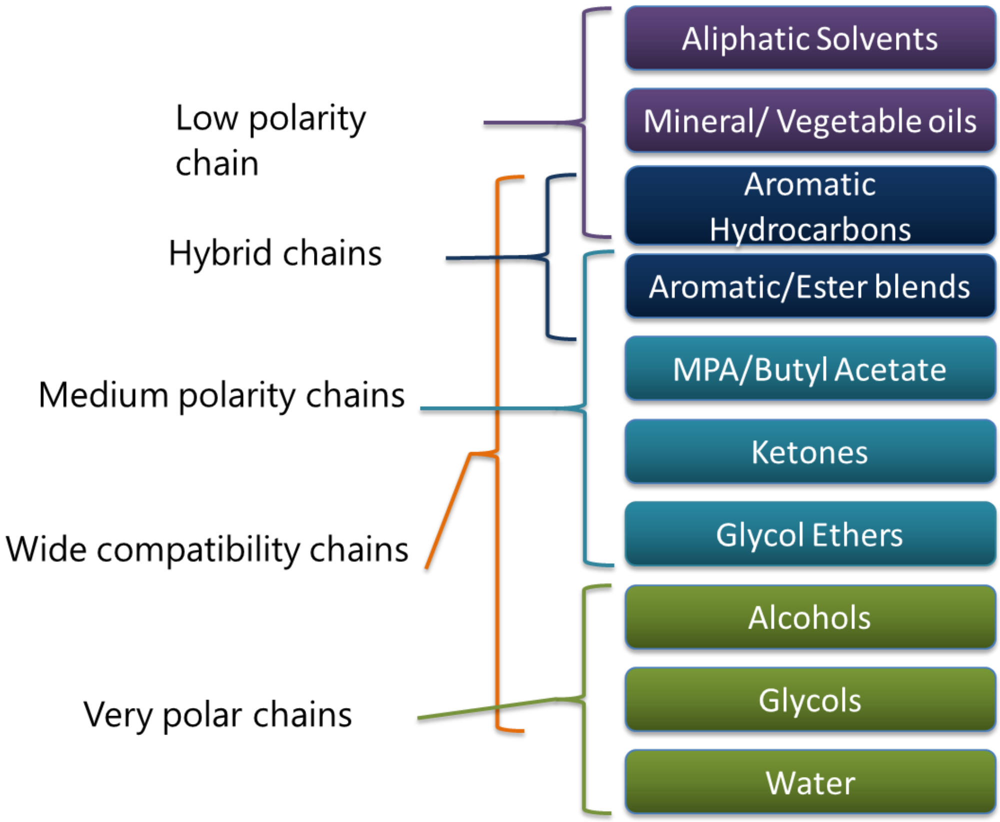
The steric stabilising chain must be compatible with the **solvent**- or it will collapse- different solvent requires different chains.

It must also be compatible with the **resin** after the solvent has evaporated.

The polarity of the monomer dictates which solvents and resins the dispersant will be compatible with.

The steric stabilising chain is the biggest part of the structure, thus the part which drives material cost. Therefore, low-cost monomers are preferred.

The compatibility of the different polarity chains with the most common solvents used in industrial applications would be as below:



The most common polymers used in dispersants with multiple stability chains are:

- Polyethers
- Polyesters/ Polylactones, homo & copolymers
- Linear and branched alkyl initiators
- Soluble Acrylics

Conclusions

The performance needs of a hyperdispersant, added to the non-performance needs, make for a complex series of requirements. Understanding the structure and make-up of a complex structure such as a dispersing agent allows the skilled chemist to design a new product using building blocks which will give the correct properties, performance, cost and regulatory profile. Lubrizol's Solsperse™ Hyperdispersants, a range of around 250 different dispersants, can offer a solution to suit the often complex needs of our customers- and we are constantly working to produce innovative solutions suitable to match the requirements of the modern Industrial Coatings sector.