Formulating and Processing Pigment Dispersions

Eyer, Kayla J.B.
American Colors, Inc.
March 2019

Pigment dispersions are widely used in the plastics and coatings industries in applications ranging from thermoset and fiberglass reinforced plastics, to paints, caulks and adhesives, to can coatings, and much more. The market for dispersions is so wide that its products must be customized to suit the needs of specific applications. For example, a water-based dispersion would clearly not be suitable for a system which needs to be able to withstand heat greater than 100° C, and a resin-based dispersion would not be suitable for a system in which the resin is insoluble. Although this customization can often complicate the formulation process, there is a simple starting point to creating any dispersion. That is, every pigment dispersion starts with three primary ingredients: a grinding vehicle, a pigment, and almost always a surfactant. The choice of these three items is where the formulation process begins.

A *dispersion* is defined to be the ultimate state of homogeneous[1] suspension of one phase with another. In this case, these phases consist of the solid (pigment) phase and the liquid phase composed of the grinding vehicle and other surfactants or additives. In order to understand dispersions more thoroughly, one must understand their components. A *pigment* is a solid-state insoluble coloring agent composed of at least one chemical compound which absorbs and reflects light in order to give the physical appearance of color. While pigments are not the only kind of coloring agent, they should not be confused with dyes, which are solid- or liquid-state soluble coloring agents. Dispersions are concerned only with insoluble coloring agents. The term *grinding vehicle*, or *carrier*, has a more complex definition, as it may refer to many different liquid phases in a dispersion. Most often the liquid phase is a resin, water, organic solvent, or some combination thereof. Some dispersions may be required to have 0% VOCs by design, while others may require volatile solvents in order to dissolve a resin or lower the viscosity of the dispersion. The choice of grinding vehicle is dependent on compatibility with the system in which the dispersion will be used as well as compatibility with the pigment(s) needed to create the desired color. The goal of the grinding vehicle is to evenly distribute pigment particles throughout the liquid system, and to provide a media through which to grind pigments into their primary particles for best color development. When a pigment is incompatible with the grinding vehicle, *surfactants* come into play. Surfactants aid in the distribution of pigment in the liquid phase, usually through hydrophobic[2] and hydrophilic[3] interactions between the surfactant molecules with the pigment particles and the surfactant

[1]**Homogeneous:** of uniform structure or composition throughout.
[2]**Hydrophobic:** lacking an affinity for water; repelling water.
[3]**Hydrophilic:** having an affinity for water; capable of interacting with water through hydrogen bonding.

molecules with the carrier. A barrier is created between pigment and carrier which results in the homogeneity desired.

There are other additives which are sometimes required in order to get preferred dispersion properties, such as dispersants with other mechanisms than surfactants, synergists, which help to improve the power of a specified surfactant, wetting agents, which reduce the surface tension between a liquid and a solid, thickeners and defoamers. These are all supplementary ingredients to the primary components of the dispersion, and can be used to improve the properties of a finished dispersion as well as the ease of processing.

For any pigment dispersion, there is a set of goals to aim for in a finished product. Aside from being the correct color, a quality dispersion has the lowest possible viscosity for the pigment loading required, is also low in VOCs, has good hiding power[4] and consistency in color, is resistant to pigment flocculation, flows well, has a stable shelf life, and is made from a simple and cost effective formula. Other factors might be specific to the application of the dispersion, like gloss, chromaticity, opacity, fastness, abrasiveness and specific chemical content. For example, a given pigment chemistry may be inexpensive, compatible with the grinding vehicle, and easy to process, but could be incompatible with the system in which the dispersion is being used. In this case, an alternative pigment needs to be found which has comparable value in the dispersion and is also compatible with the application. It can be challenging to achieve all of the goals of a quality dispersion and can take a significant amount of time and thought during development. A design of experiment (DOE) is often useful for optimizing the formulation while minimizing the number of trials needed.

One of the challenges with processing a dispersion is stabilization of the pigment in its primary particle state. In its dry form, a pigment *aggregates* into groups of primary particles connected at their face through intermolecular forces[5]. Particles which are not necessarily covalently[6] or ionically[7] bound are drawn to each other through forces such as hydrogen bonding[8], ion-dipole[9], and dipole-dipole[10] interaction. The surface area of these aggregates is much larger than the surface area or the primary particles, but the surface area of an aggregate is much lower than that of the sum of its primary particles. *Agglomerates* are similar to aggregates, but are groups of primary particles connected at their edges and corners through weaker attractions to each other. Weaker still is the attraction of primary particles to each other in *flocculates*.

---

[4]**Hiding power:** the ability of a dispersion to obscure the surface upon which it is applied.
[5]**Intermolecular forces:** forces of attraction or repulsion between neighboring molecules in a system.
[6]**Covalent bond:** sharing of a valence electron pair by two atoms.
[7]**Ionic bond:** transfer of valence electron between two atoms.
[8]**Hydrogen bonding:** an electromagnetic attraction between hydrogen and electronegative atoms such as nitrogen, oxygen, or fluorine; the strongest intermolecular force.
[9]**Ion-dipole:** an electrostatic attraction between an ion (charged atom or molecule) and a molecule which had a dipole (separation of positive and negative charge)
[10]**Dipole-dipole:** an electrostatic attraction between two molecules which have dipoles.

In order to disperse a pigment in a dispersion and develop its color fully, it must be processed in the liquid phase through a series of mechanical methods of breaking apart aggregates, agglomerates and flocculates. This procedure is called grinding, and will vary in ease with different pigments. Some pigments can be ground into primary particles by applying heat and shear with an overhead mixer. This is referred to in the dispersion industry as high-speed mixing. Other pigments require greater amounts of shear, which can be obtained with a horizontal mill, roll mill, or ball mill. Each of these machines use mill media or rolling gears which force pigment agglomerates through small spaces between the media (or between the gears) resulting in a mechanical breakdown of pigment into smaller and smaller particles. Some pigments require only one pass through a mill, while others require multiple passes to obtain the desired grind. Ease of dispersion of a pigment into the grinding vehicle is dependent not only on pigment chemistry, but also on the process through which a pigment is produced and surface treated. The only way to really know whether a pigment requires a significant amount of processing in the grinding vehicle is to try dispersing the pigment and check the grind along the way.

Once a pigment is broken down into its primary particles, intermolecular forces are responsible either for maintaining this dispersion or allowing flocculates and aggregates to reform. The best way to stabilize a pigment in a grinding vehicle is with a surfactant. Surfactants are most commonly composed of molecules with one hydrophobic end and one hydrophilic end. The hydrophilic end is polar[11] and has charges which are compatible with the dipole moments[12] of certain pigments. These ends anchor to a pigment particle, surrounding it and creating a barrier from the carrier. The hydrophobic end is nonpolar[13] and is compatible with nonpolar carriers. In a water-based or other polar grinding vehicle system, the roles of the hydrophobic and hydrophilic ends are reversed. The structure formed by the surfactant molecules and the pigment particle is called a micelle, and is similar to the structure or the cell membranes surrounding the cells of any living beings. Other types of surfactants utilize the functional groups on pigment particle surfaces such as hydrogen bonding sites, and are more specific to individual pigment chemistries.

The pigment dispersion industry is sourced with innumerable varieties of pigments, resins, solvents, surfactants, and other additives. Coupled with the variety of processing methods, it can be difficult to uncover an ideal dispersion for a given application. However, this variety also accounts for the broad scope of applications in which pigment dispersions can be used. An understanding of the formulating process is vital to arriving at the correct formulation for any given application.

---

[11] **Polarity:** separation of charge due to a difference in electronegativity.

[12] **Dipole moment:** separation of positive and negative charge which may be permanent in a molecule or induced by an external electric field.

[13] **Nonpolar:** exhibiting no separation of charge.