Formulating Fundamentals for Coatings and Cleaners

Summary

Solvents are essential formulation ingredients for many coating and cleaning jobs. Without them, paints and cleaning products would simply not perform as well. However, choosing the appropriate solvent or solvent blend for a particular application is often not easy. Many variables must be considered, and the choice is system-dependent. For example, reformulating an existing product is not as simple as substituting another — even similar — solvent. To use a new solvent, a product typically needs to be completely reformulated to maintain desired performance attributes. Because formulations are complex, and reformulations could result in a poorer-performing product, it is wise for formulators to work with their solvent suppliers to find the best solvent system for the desired application.

This article is intended to introduce solvent users, formulators and regulators to the basic principles of how solvents work in consumer and industrial products. It is not intended to address specific formulation choices; as the article notes, complex decisions are made through consultation between the solvents supplier and product formulator. It is not intended to provide an exhaustive discussion of all the factors that may affect formulation decisions.

Introduction

Solvents improve the effectiveness and performance of hundreds of home and business products. They are essential ingredients in many coatings and cleaners. Solvents help paint flow and form smooth surfaces, help inks dry, help cleaning products work better and support the production of pharmaceuticals — to name only a few examples.

> **Formulating**: "The selection of components of a product formula or mixture to provide optimum specific properties for the end use desired. Formulation by experienced technologists is essential for products intended to meet specifications or special service conditions." … *Hawley's Condensed Chemical Dictionary*

However formulating isn't simply a matter of adding a certain amount of any solvent to an automotive coating or household cleaner. The function of the solvent in the final formulation and performance of the product — as well as regulatory requirements and safety are all considerations when making formulation decisions. For optimal performance, the right solvent or solvent blend must be matched to the specific application.

It can be challenging to find the right solvent or solvent blend for a specific use. This article discusses some of the key issues — and provides an introduction to some of the factors —to be considered when selecting solvents for formulating coatings and cleaners.

Solvent Application

To begin developing a solvent system for a formulation, a formulator first considers what the solvent is being asked to do in the formulation and the desired qualities of the formulated product. The questions are basic but vital. What is the solvent being used for? What is its function in the product? How will it be applied in the process? Some key questions are:

- What is the intended end-use?

An automotive coating, a household paint, a household cleaner, a metal parts cleaner?

- What are the essential ingredients?

Resins, pigments, solvents, surfactants, etc.

- What are the limitations, if any?

Dry-time requirement, odor, health and safety, etc.

- Are there any special considerations?

Air-dry versus baking applications.

- Can a balance be achieved by taking into account the complexity of ALL the variables?

Other factors may be relevant to the formulation decision, such as the interaction of the solvent with other materials in the product or the advantages and disadvantages of various solvents for the application. There will always be tradeoffs. For example, a particular solvent may dissolve a resin very effectively, but dry too slowly for the application. Or a certain solvent may release little or no volatile organic compounds (VOCs), as in a low VOC paint, but the paint may require more frequent application because the paint is less durable and washable.

With knowledge of how the solvent — and final formulation — will be used, a formulator can begin thinking about other factors that will affect the selection of solvents for the formulation.

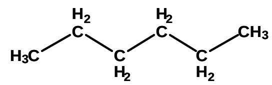
Solvent Selection

Solvent Type is one of the first things to consider when choosing a solvent for a formulation. Solvents can be organic (contain carbon, such as rubbing alcohol) or inorganic (do not contain carbon, such as water). Organic solvents are further classified by chemical structure, as shown in the box illustration above. Most organic solvents used in the United States are hydrocarbon or oxygenated solvents, and those are the main focus of this article. Chlorinated solvents also are organic solvents, but are not included in this article because of their limited use in these applications.

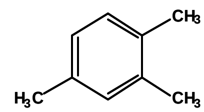
Hydrocarbon and Oxygenated Solvents

Hydrocarbon Solvents

Aliphatic

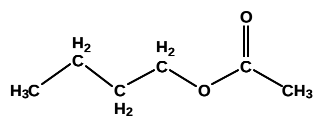


Aromatic

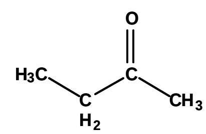


Oxygenated Solvents

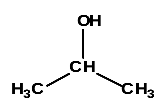
Ketones



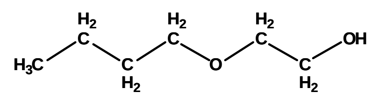
Esters



Alcohols



Glycol Ethers/Esters



Since solvents are used to dissolve other substances — and since a basic principle of how solvents work is "like dissolves like" — the solvent of choice will almost always be one that is chemically similar to the material being dissolved.

For example, although water dissolves many substances, it does not dissolve oil or grease. Thus, dishwashing cleaners contain solvents that are chemically similar to oil and grease so that these materials can be dissolved and removed from dishes.

Health, Safety, and Environment (HSE) issues, including compliance with state and federal regulations, are important considerations before making a formulation decision. Solvents should be handled carefully to minimize risks of fire or explosion, and they should be used in adequately ventilated areas. HSE issues include:

- Volatile Organic Compound (VOC) Content
- Flammability
- Toxicology Profile
- Threshold Limit Values
- Photochemical Reactivity
- Biodegradability
- Hazardous Air Pollutant Profile
- Odor

VOC considerations are especially important. For example, with regulatory mass-based VOC limits for coatings, VOC content can be reduced by (1) using VOC-exempt solvent(s), (2) choosing the most efficient solvent or solvent blend that provides other necessary coating properties, or (3) reducing the molecular weight of the resin (this often requires less solvent, but can result in inferior coating performance). Thus, when choosing the right solvent, it is not always possible to find a non-VOC replacement for a VOC-solvent. The interactions of all the materials in the final product are complex, and VOC-solvents may be needed to achieve the required formulation performance characteristics.

The formation and accumulation of ozone (primary component of smog) is a complex process involving heat, sunlight, NOx (such as from auto exhaust) and VOCs. A VOC's potential contribution to ozone accumulation depends largely on its "photochemical" reactivity, and VOCs vary greatly in that regard. By using products with low photochemical reactivity, a formulator sometimes can meet performance requirements and contribute to improved air quality. Use of VOC solvents with lower photochemical reactivity lowers the "ozone-creation potential" of a formulated product.

Solvent Performance is one of the key factors in choosing a solvent for a coating or cleaner. Solvent selection is system-dependent — the solvent must meet both the performance criteria of the product and be suitable for the desired method of application. Solvent performance is characterized by the physical properties of the solvent itself, as well as by the resulting physical properties of the final coating or cleaner (e.g., dry time). This article separately reviews formulation considerations for coatings and cleaning products in terms of the key physical properties that impact product performance.

Solvent Performance in Coatings

Solvency is one of the most important physical properties since it defines a solvent's ability to dissolve a resin in a coating and decrease the solution viscosity. The key concept is "like dissolves like." Thus, aliphatic solvents will tend to dissolve "hydrocarbon-like" resins while polar (e.g., oxygenated) solvents may be required to dissolve other resins, such as polyesters, acrylics and polyurethanes.

One of the key measures of solvency is coating **viscosity**. Viscosity is a measure of a fluid's resistance to flow. The most efficient solvent provides the lowest viscosity at a particular total solids level. Or at a particular viscosity, the desired solvent will provide the highest total solids or require the least amount of solvent.

Solubility parameters are used to characterize solvents and predict which solvents will dissolve what resins. They help guide a formulator and narrow the choices from the myriad of potential solvents and blends available. Since "like dissolves like," solubility parameters take into account such things as solvent polarity and hydrogen-bonding to determine which solvents are more like the material that needs to be dissolved.

Relative Evaporation Rate (RER) is a measure of how fast a solvent evaporates. Solvents work by dissolving resins or polymers to produce a useable liquid, then evaporating after application to leave a coating. n-Butyl Acetate is typically used as a reference, with its RER set at 1 or 100. Faster evaporating solvents are typically used in air-dry applications, while slower evaporating solvents are used in baking applications.

Coating formulations often include several solvents that evaporate at different rates. For example, a typical spray application paint formulation may include fast, medium, and slow evaporating solvents. The fast evaporating solvent provides a lower initial paint viscosity for easier application (good atomization of the spray), while allowing a higher viscosity after application (after the fast evaporating solvent quickly disperses) to help prevent dripping and sagging. The medium evaporating solvent provides a more controlled release to help prevent film defects arising from too rapid solvent evaporation. And the slow evaporating solvent, the last to leave the system, finalizes flow and leveling and thus provides a uniform film thickness which impacts the final appearance and the final mechanical properties (such as adhesion).

The ***Vapor Pressure*** and ***Boiling Point*** of a solvent are typically not major considerations for coatings (RER is the determining property). Vapor pressure, the pressure at which a vapor is in equilibrium with its liquid, is directly proportional to RER. Boiling point, the temperature at which a liquid changes to a gas at atmospheric pressure, is inversely proportional to RER.

Flash Point is the temperature at which a liquid gives off enough vapor to form an ignitable mixture. It is an important safety consideration that affects the application of the solvent, including selection of equipment and facilities for manufacturing and applying the formulation. Flash point is inversely proportional to RER.

Density is the weight of a solvent divided by its volume, typically measured as Lbs/Gal or gms/L. The importance of density is its effect on the VOC content of formulations. Solvents with greater densities contribute to higher VOC content, everything else being equal.

Electrical Resistivity is a critical property for solvents used in coatings applied by electrostatic spray, a process that atomizes and charges paint particles, increasing their attraction to metal parts and decreasing paint usage and emissions.

Viscosity is a measure of a fluid's resistance to flow. However, the solvency of the solvent has a greater impact on the formulation viscosity, since solvents with higher solvency decrease formulation viscosity by dissolving the resin.

Surface Tension is the force per unit length in the surface of a liquid. Low surface tension allows for enhanced substrate wetting, improved sprayability, and reduced number and severity of coating defects.

Solvent Performance in Cleaning Products

Formulation of cleaning products depends on the type of dirt or soil to be removed, the type of substrate that needs to be cleaned, and the method to be used for cleaning. Solvents are used in cleaning products to dissolve water-insoluble soils, to keep water-soluble soils suspended so they can be rinsed away, and to control evaporation rate to match the requirements of the application.

Coupling and ***Solvency*** are important for binding or dissolving soils for removal. For non-water-soluble soils, the solvent must dissolve the soil, and solubility parameters are used to help select solvents. For water-soluble soils, the solvent helps suspend the soil so that it can be removed and washed away. Water-miscible solvents (like glycol ethers) are used to couple organic soils with water while hydrocarbon solvents are used for heavy-duty degreasing applications such as engine degreasers and metal parts cleaners.

Surface Tension is important for wetting the soil and cleaning surface. Solvents with low surface tension provide improved soil and substrate wetting, allowing effective soil penetration and dissolution.

Relative Evaporation Rate (RER) is important for cleaning products as well as for coatings. Solvents in cleaning products evaporate while the cleaner dries on the surface being cleaned. A fast-evaporating solvent is usually desired, but if the solvent evaporates too quickly, the coupling or solvency, and thus the effectiveness of the cleaning product, are reduced. The end use of the product will determine the optimum balance between evaporation rate, cleaning time, and flash point.

Shelf Stability is a measure of how long a cleaning formulation maintains its original (manufactured) physical properties when stored. Shelf stability is of particular concern for consumer products where shelf time can be considerable and the product may go through large temperature swings during transit and storage. Shelf stability considerations include the compatibility and stability of the solvent, over various periods of time, with other components of the formulation, such as fragrances, dyes, and surfactants.

Conclusion

Solvents are important components in coatings and cleaners, and selecting the optimal solvent or solvent blend for a formulation is complex. Consideration of system, application, solvent type, and HSE often narrows the choices considerably, but solvent performance, based on the physical properties of the solvent and the final formulation, is typically used to make the final selection. Thus, no matter which solvent or solvent blend is chosen in the final formulation, there are tradeoffs between all these important variables. Although it would be nice to simply add a mild solvent like water to every formulation, it is simply not feasible. Consider a relatively benign application like household dishwashing, where the main solvent is water but other cleaners are still required for adequate cleaning. Thus, formulation is a complex process, requiring solvent suppliers to work with downstream users to find the best solvent system for a particular formulation.

American Solvents Council

The American Solvents Council of the American Chemistry Council includes producers of oxygenated and hydrocarbon solvents. The ASC was created to address health, safety and environmental issues that affect producers, distributors, and users of modern hydrocarbon and oxygenated solvents. The ASC supports scientific research, participates in regulatory activities pertaining to solvents, and works to ensure solvents continue to be recognized as important components of a wide range of products that make our lives safer and healthier while meeting the challenges of today's environmentally conscious world. For more information about this article, or the ASC, please visit us at www.americansolventscouncil.org.

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