Modeling of Total Solar Reflect

ance as a Formulation Tool

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New uses for solar heat management (SHM) coatings are expanding in demand beyond the traditional building products markets. New areas of application, including transportation, consumer comfort, and safety, are joining energy conservation where near infrared (NIR)-reflective pigments can add value.

What if the formulation process for these coatings included modeling the reflectance behavior of the surface before a drop of paint was made? The best candidates for the application could be chosen—minimizing trial, error, and cost—in the development process.

This article outlines the formulation process for an SHM coating utilizing proprietary modeling software to predict the total solar reflectance (TSR) of a trial coating. Examples illustrate the influence of formulation and substrate on predicted and measured TSR values.

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INTRODUCTION

Every industry, including the coatings industry, is under pressure to increase productivity. The emphasis remains on doing more with fewer resources in less time. One way to accomplish this is to make use of modeling software. Modeling an important property of a coating can shorten the development cycle and allow formulators to reach an acceptable solution sooner.

Some coating properties lend themselves well to simple models such as the relationship between nonvolatile percentage and volatile organic compound (VOC) content. Other properties, like color matching, require complex mathematical representations.

In this article, we illustrate how modeling the surface property of TSR can shorten the development cycles for coatings used for SHM applications. Two examples will demonstrate how the best coatings candidate for further development can be chosen to achieve surfaces with high solar reflectivity.

IMPORTANCE OF SOLAR REFLECTANCE

The energy sustaining life on earth (including its human inhabitants) is derived from the sun, whether it is utilized directly like photosynthesis and solar panels or indirectly in the form of fossil fuels. Life on earth is possible because of the sun's energy. However, the sun is not always beneficial to mankind's endeavors, and, in some situations, the energy of the sun needs to be managed.

When the surface of an object is exposed to sunlight, three things can happen to the solar energy—energy can be transmitted, reflected, or absorbed. When energy is absorbed, it is converted to heat, and the surface temperature rises. Conductivity transfers heat to the entire object, and convection can heat the interior of a hollow object.

From tropical to temperate regions around the globe, energy is expended, cooling buildings and vehicles. The more solar energy absorbed by a structure, the more energy needs to be used to cool the interior to a comfortable temperature. Concentrations of man-made structures often absorb more solar energy than natural areas, leading to the urban heat island effect around large cities. Reflecting a portion of that solar energy can reduce the energy demand for cooling. Some manmade materials are heat sensitive, but are still used in applications where they are exposed to sunlight. If solar energy is absorbed by these objects, they may be physically damaged or lose strength. If a dark-colored object remains in the sun for too long, it can become literally too hot to handle and uncomfortable or unsafe to touch. Specialized coatings formulated to reflect solar energy can help manage these effects.

THE COATINGS FORMULATION PROCESS

As in any product development process, there is a cycle-to-coatings formulation, which usually starts with color and performance standards that need to be met and progresses from there. Often multiple trial coatings are formulated and made in the lab followed by preparing test sample panels that are tested with the results guiding the next round of samples. An increase in the number of target parameters further complicates the process since frequently changing a test formula to improve one property can degrade the performance of another. Not all performance properties lend themselves to the use of models to predict results. Properties that cannot be accurately modeled are optimized through experimentation. Examples of these are corrosion resistance and weathering as measured by chalk and fade resistance. General knowledge and experience can guide the formulator in these areas, but accurate predictive models of these properties are not commonly used.

MODELING TSR AS A FORMULATION TOOL

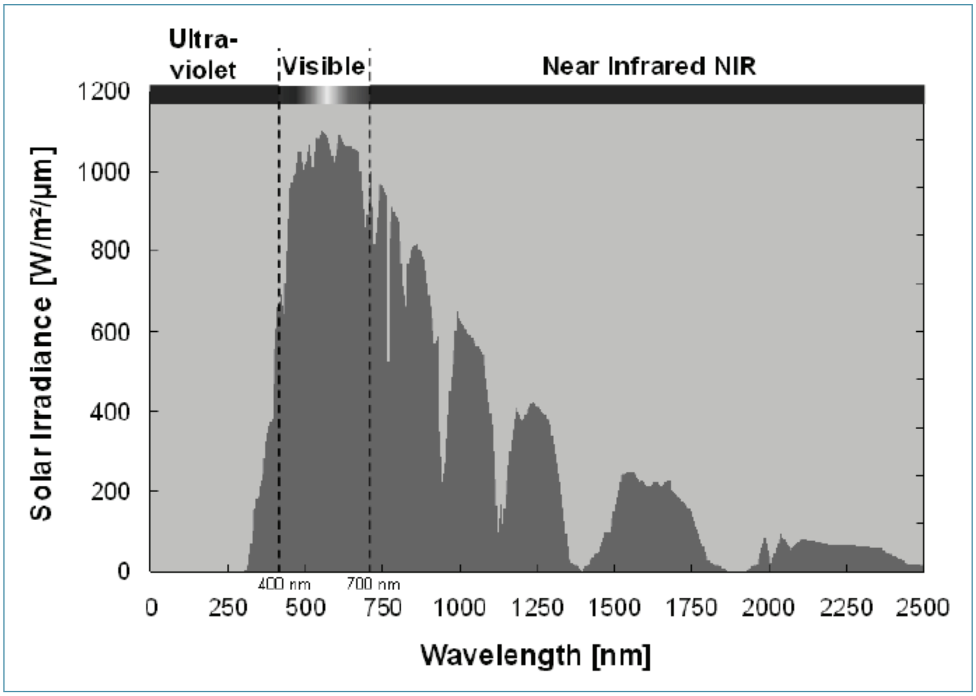
When one of the properties called for in a coating is a specific or minimum value of TSR, the formulation process is further complicated. Generally, TSR must be measured experimentally using a standard method. The need for experimental data requires sample coating preparation and application before the best candidates are chosen for further application and performance testing to optimize the formulation.

Applications used to predict formulation properties—including weight and volume nonvolatiles, VOC, and even color match—are commonplace in the coatings development lab. Formulation changes can be modeled with these types of software to optimize coatings properties before making physical samples for testing. The development cycle is streamlined by using modeling to predict the effect of changing one variable to another.

Software designed to determine the reflectance properties of surface coatings, whether limited to the visible portion of the spectrum (color matching) or prediction of TSR, is based on the work of Paul Kubelka and Franz Munk.[1] Kubelka and Munk first published their work concerning the calculation of light scattering from opaque paint films in 1931. The total solar reflectance value for a pigment combination is calculated from the absorption and scattering coefficients for the individual pigments over the wavelength range from 300 to 2500 nanometers.

The solar energy reaching any point on the earth's surface varies with the seasons and the time of day as well as elevation and weather conditions. Standard models of solar irradiance were established to quantify the distribution of solar energy and enable calculations of its effects.

FIGURE 1—Solar irradiance according to ASTM G 159 (198), air mass 1.5[2]. Standard solar irradiance at the earth's surface corrected for atmospheric absorbance.



FACTORS INFLUENCING THE SOLAR REFLECTANCE OF A COATED SURFACE

Figure 1 shows the solar irradiance broken down into three regions: ultraviolet, visible, and near infrared (NIR). Each of these categories must be managed in a different way to achieve the desired TSR of the surface.

Since the ultraviolet region of the solar spectrum only accounts for 3% of the energy striking the earth from the sun, it plays a minor role when calculating the TSR. Although UV radiation can have many effects on a coating, ultraviolet energy absorption contributes very little to the temperature increase of the surface.

The visible region of the spectrum is where the perception of color is grounded. When matching color, the visible reflectance is determined by the color requirements. This region accounts for approximately 39% of solar energy reaching the earth's surface, but one cannot significantly increase the reflectance profile in this region without negatively affecting the color match.

At 58%, the majority of solar energy reaching the earth's surface is in the NIR region. The greatest effect on TSR can be realized by altering the reflectance of the surface in the NIR.

COLOR AND PIGMENTATION

The visible portion of the solar spectrum should be managed with the goal of matching the reflectance spectrum of the target color standard. A close correlation to the visible reflectance of the target color will help to achieve a color match that is consistent under varied lighting conditions. The reflectance in the visible region depends largely on two factors: the absorbance of light by the pigment and the scattering of light by the pigment. Absorbance of light is the main determining factor for the color seen by the eye, while scattering largely influences the opacity or hiding of the coating.

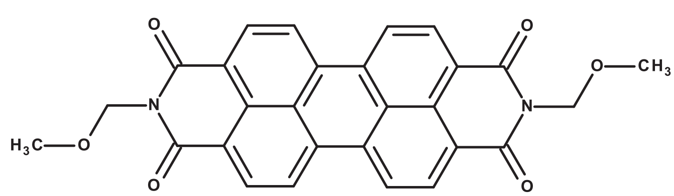
Modeling software to help match color is commonly used in the coatings industry. There are both proprietary and commercially available applications that can take visible reflectance spectral (color) data and provide possible pigment combinations to match the color.

The main consideration when color matching coatings intended for use in SHM applications is the influence the pigments used to match the visible reflectance spectrum will have on the reflectance spectrum in the NIR. A primary purpose here is to illustrate the use of software that can model the TSR to guide the choice of the pigments used in color matching.

The most important principle to follow when formulating high TSR color matches for coatings used in SHM is to replace carbon black pigments with black pigments that do not absorb NIR radiation. These are often called functional black pigments. There are two main Colour Index number pigments used as functional black pigments. The first is Pigment Brown 29 (PBr 29), which is an inorganic mixed metal oxide of iron and chromium. PBr 29 strongly reflects NIR radiation in the region from 1100 to 2500 nanometers.

The second important functional black pigment is Pigment Black 32 (PBk 32) (*Figure 2*). This organic pigment, also known as perylene black, is highly transparent to NIR radiation from 700 to 2500 nanometers. This transparent behavior offers a unique way to obtain high solar reflectance properties from dark colored surfaces.

FIGURE 2—Structure of Pigment Black 32 (PBk 32), an NIR-transparent perylene black pigment used to make high solar reflectance coatings.



PBk 32

TABLE 1—Predicted TSR Value for Gray Coatings Made with NIR-Reflective Black Pigment[a]

GRAY COATING L VALUE	PREDICTED TSR OVER WHITE SUBSTRATE (%)	PREDICTED TSR OVER BLACK SUBSTRATE (%)	RATIO OF TIO_2 TO NIR-REFLECTING BLACK
97	86.0	79.6	100/0
55	41.1	38.6	77/23
45	33.5	31.7	55/45
35	27.8	26.6	25/75
28	24.7	23.7	0/100

(a) The table shows that the substrate effect is minimal when using NIR-reflective pigments.

TABLE 2—Predicted TSR Value for Gray Coatings Made with NIR-Transparent Black Pigment[a]

GRAY COATING L VALUE	PREDICTED TSR OVER WHITE SUBSTRATE (%)	PREDICTED TSR OVER BLACK SUBSTRATE (%)	RATIO OF TIO_2 TO NIR-TRANSPARENT BLACK (PIGMENT BLACK 32)
97	86.0	79.6	100/0
55	51.6	31.3	90.5/9.5
45	47.2	26.6	79.5/20.5
35	43.1	21.1	55/45
25	38.8	10.6	0/100

(a) The table shows the effect the substrate can have on the predicted TSR values when NIR-transparent pigments are used to make a gray coating.

SUBSTRATE INFLUENCE

The coating is not the only component influencing the solar reflectance of a surface. Near infrared radiation can penetrate a coating and be absorbed or reflected by the substrate. This is possible because of the longer wavelength of the NIR radiation. As the wavelength of the impinging radiation increases relative to the particle size of the pigment, the scattering efficiency of the pigment is reduced. *Table 1* lists the predicted TSR of a series of gray coatings with the corresponding CIELAB Lightness (L) values for coatings containing NIR-reflective PBr 29. In *Figure 3,* the data from *Table 1* is represented graphically, illustrating the minor effect of substrate on TSR when a coating uses NIR-reflective pigments.

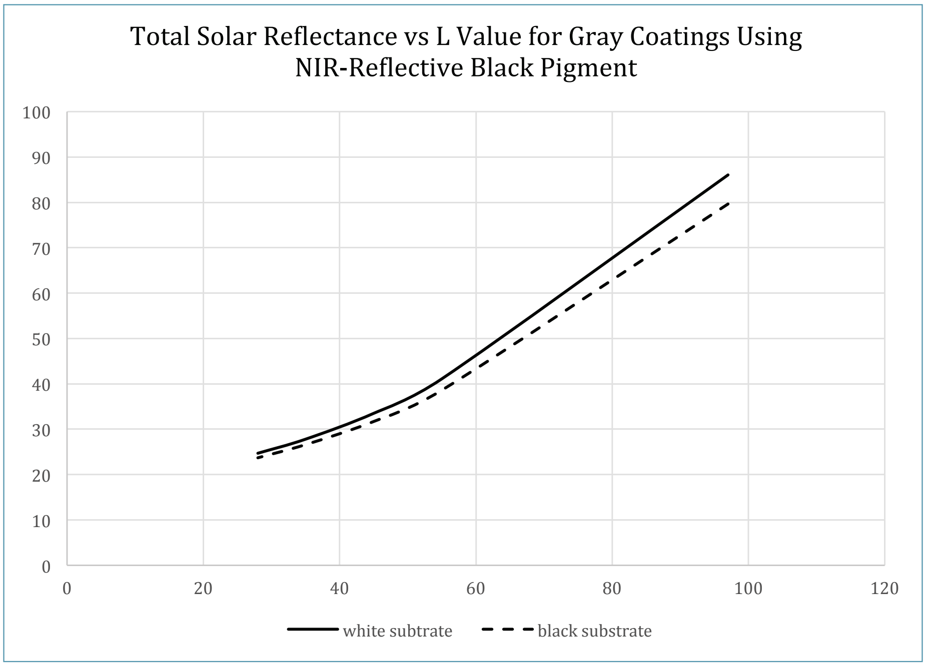
To accurately model the solar reflectance of a coated surface, the influence of the substrate NIR reflectance must be taken into account. Substrate influence can even be used to increase the TSR reflectance of a surface. By using pigments that are NIR transparent, that neither absorb nor reflect NIR, in a coating over a highly solar reflective substrate, surfaces with high TSR values can be achieved. *Table 2* lists the TSR and L values for a series of gray coatings made with NIR-transparent PBk 32. In *Figure 4,* the graphic depiction of this data shows the increased influence of substrate color on the TSR value.

EXAMPLE: HEAT-SENSITIVE POLYMER BUILDING PRODUCTS

An established application for SHM coatings is on building products fabricated from heat-sensitive polymeric materials. Here, the goal is not reduction in energy use directly but, rather, to enable a selection of a broader range of materials and provide a selection of colors to the consumer.

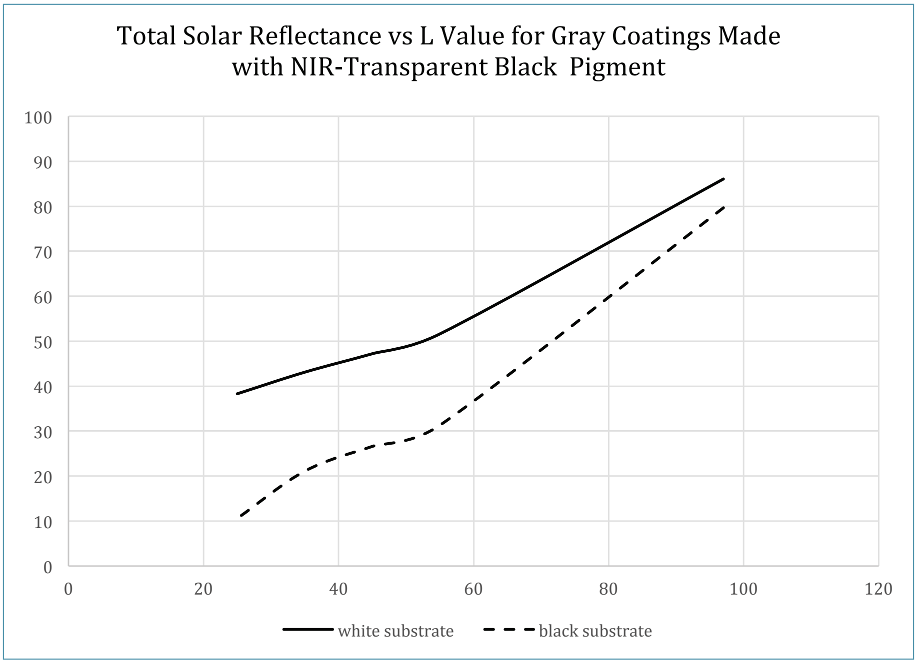
Polyvinylchloride (PVC) is well suited to forming a window frame lineal. The heat deflection temperature of many extrusion grades of PVC is approximately between 65.6°C and 71.1°C (ASTM Method D648, 256 psi). This test measures the temperature at which a

FIGURE 3—Substrate influence for an NIR-reflective coating.[a]



(a) Plotting the predicted TSR value over white and black substrates vs the L value of the gray coatings shows that the substrate influence is minimal when using NIR-reflective functional black pigments.

FIGURE 4—Substrate influence for an NIR-transparent coating.[a]



(a) As the L value decreases, the influence of the substrate on TSR results is more pronounced when NIR-transparent functional black pigments are used to make gray coatings.

TABLE 3—Predicted and Measured TSR Values over White Vinyl Substrate[a]

PIGMENT COMPOSITION	NIR -TRANSPARENT PIGMENTS (%)	NIR-REFLECTIVE PIGMENTS (%)	CONVENTIONAL PIGMENTS (%)
PIGMENT BLACK 32 PERYLENE BLACK	13.9	—	—
PIGMENT BROWN 29 IRON CHROMIUM (III) OXIDE	—	65.9	—
PIGMENT BLACK 7 CARBON BLACK	—	—	7.5
PIGMENT WHITE 6 TITANIUM DIOXIDE	—	—	17.2
PIGMENT YELLOW 151 BENZIMIDAZOLONE	65.8	12.4	—
PIGMENT RED 264 DPP RUBINE	20.4	—	—
PIGMENT RED 254 DPP RED	—	21.6	9.9
PIGMENT ORANGE 73 DPP ORANGE	—	—	65.4
PREDICTED TSR VALUE	43.8	33.3	5.6
MEASURED TSR VALUE	43.6	27.8	6.4

(a) The data shows that the highest TSR value over white vinyl substrates are obtained when using NIR-transparent functional black pigments.

test specimen deflects 0.25 mm under the specified load. Heat deflection temperature correlates to maximum service temperature in applications that require close dimensional tolerances such as vinyl window frames. A dark-colored window frame in direct sunlight can easily reach this temperature through solar energy absorbance. If a dark-colored window frame is the architect's choice, an SHM coating is necessary to ensure dimensional stability.

A vinyl window frame profile is a classic example of using an NIR-transparent coating over a solar energy reflective substrate. White pigmented PVC compounds are commonly used for extruded window frames. This substrate has a high TSR value. Applying an NIR-transparent color coat over the white substrate can yield a surface with higher TSR values than an NIR-reflective coating.

The first step is to determine the pigments required to match the color or match the reflectance in the visible portion of the solar spectrum as closely as possible. Color matching software will often suggest several combinations of pigments capable of achieving this. Some combinations, such as those containing carbon black pigments, can be rejected immediately. An even better approach is to exclude carbon black from the color matching process, if possible.

In *Table 3*, three acceptable color matches for a dark brown architectural color popular for window frames (RAL 8017) were determined using color matching software. Each match belongs to one of three groups: matches using NIR-transparent pigments (examples of structures in *Figure 5*), matches using NIR-reflective pigments, and those using conventional pigments, including carbon black. These matches were modeled over the specified substrate—a white, rigid PVC plaque commonly used for extruded window frames. The pigment loading of the coating models were constructed to visually hide the difference between white and black surfaces at a dry film thickness of 50 microns.

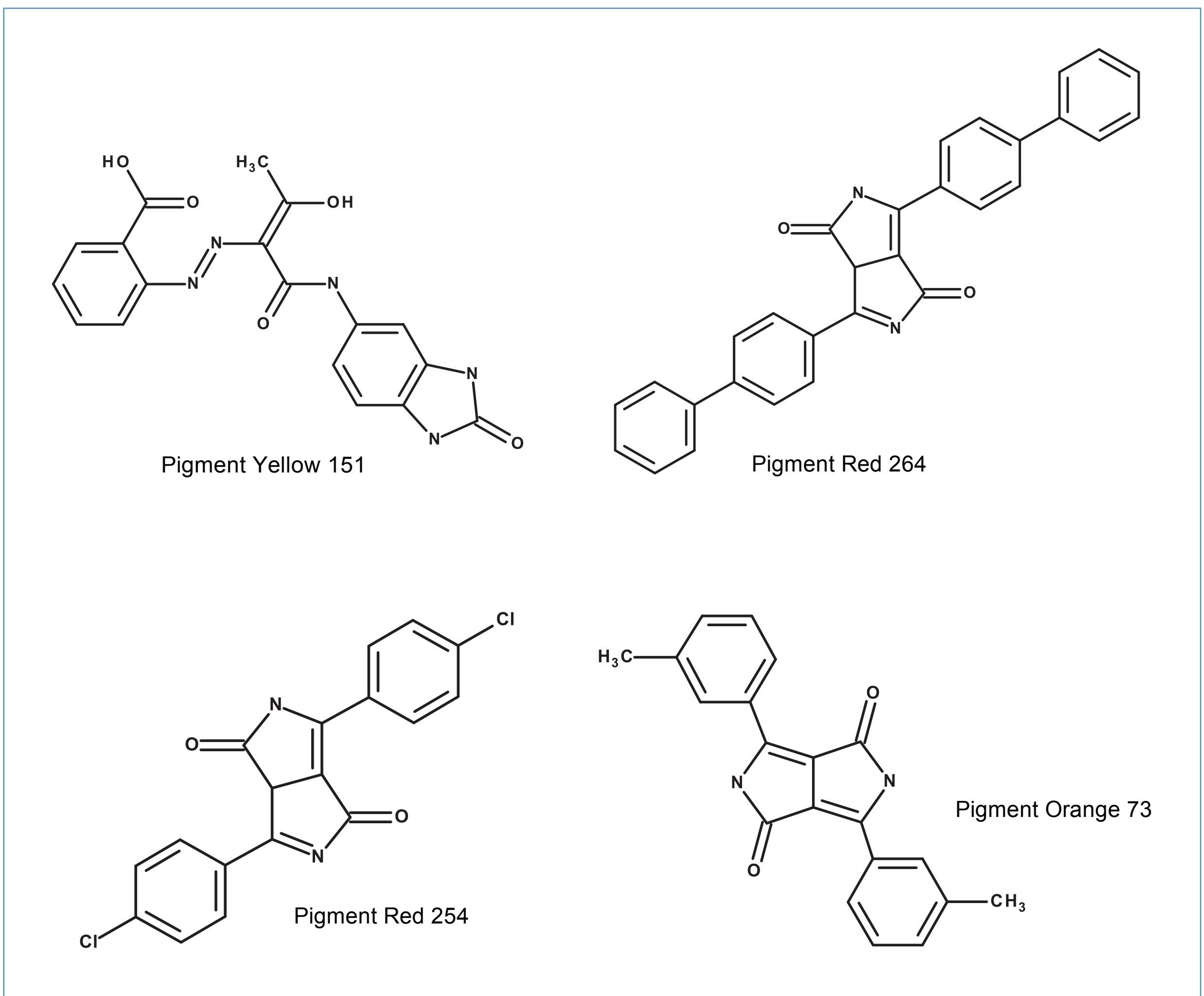
The highest TSR value is achieved by using NIR-transparent pigments in this case. Not every application can take advantage of a NIR-reflective substrate like white vinyl. In those cases, a formulation containing NIR-reflective coatings will give the best results since the TSR is less dependent upon the reflective properties of the substrate. If possible, an NIR-reflective (white) primer or mid-coat may be used to provide a highly NIR-reflective substrate. Using a solar reflectance model which accounts for substrate reflectance allows the simulation of a multi-coat system without experimentation. This allows concentrating development efforts on the trial formulas with the greatest chance of success.

EXAMPLE: HEAVY EQUIPMENT GRAB HANDLE

Sometimes an SHM surface is required for reasons other than energy management or protecting a heat-sensitive material. Comfort and safety concerns may require a lower surface temperature for an object in direct sunlight. Safety grab handles on heavy equipment typically used for mining and construction may be finished in a dark or black color to contrast with a lighter color used for the main body of the equipment to make them easy to see. In this case, RAL 9005 was chosen as the target color.

Rather than saving energy or preventing distortion of a heat-sensitive material, the goal is to reduce the surface temperature of the handle to a comfortable level. This is driven by two factors: operator comfort and proposed regulations, which specify the peak surface temperature for safety rails and grab handles. For this application, another property governed by solar reflectance is important. This is the heat build-up (HBU). The HBU is the temperature increase above ambient the surface attains when exposed to a specified NIR source.

FIGURE 5—Structures of organic pigments.[a]



(a) The figure illustrates the structure of the organic pigments used in addition to functional black pigments to match RAL 8017 in this example.

TABLE 4—Predicted and Actual TSR and Measured HBU Values over Bare Steel and White Primed Steel

PIGMENT COMPOSITION	NIR-TRANSPARENT PIGMENTS OVER WHITE PRIMED STEEL	NIR-TRANSPARENT PIGMENTS OVER BARE STEEL	NIR-REFLECTIVE PIGMENTS OVER BARE STEEL	CONVENTIONAL PIGMENTS OVER BARE STEEL
PIGMENT BLACK 32 PERYLENE BLACK	73.0%	73.0%	55.8%	—
PIGMENT BROWN 29 IRON CHROMIUM (III) OXIDE	—	—	43.0%	—
PIGMENT BLACK 7 CARBON BLACK	—	—	—	36.5%
PIGMENT WHITE 6 TITANIUM DIOXIDE	27.0%	27.0%	1.2%	—
PIGMENT YELLOW 42 YELLOW IRON OXIDE	—	—	—	63.5%
PREDICTED TSR VALUE	41.7%	27.0%	22.3%	4.3%
MEASURED TSR VALUE	37.8%	19.2%	21.7%	4.9%
MEASURED HBU	15.2°C	27.1°C	22.8°C	32.3°C

Three acceptable color matches listed in *Table 4* were determined and modeled to predict the TSR values for each. Pigment loading was again set to achieve visual hiding of the difference between black and white substrate at 50 microns.

For an application over steel, the lowest HBU correlates to the highest TSR values. Using a highly solar reflective primer under the NIR-transparent black topcoat gives the lowest HBU.

HBU is a property that does not lend itself easily to mathematical modeling due to the many factors involved. The absorption of solar energy is the first step in a chain of events that leads to an increase in temperature of an object. Other processes that occur after the initial energy absorption such as heat conduction and radiative heat loss contribute to the HBU of an object. However, HBU is inversely proportional to TSR, and a prediction of TSR can be a deciding factor when selecting candidates for coatings to reduce the HBU of an object. Modeling can be used to investigate the relative benefits of each approach to a higher TSR surface. The advantages and disadvantages of each system with regards to performance, complexity of application, and cost can be considered to find the best way to meet the expectation of the end user.

CONCLUSION

Software applications that mathematically model the total solar reflectance (TSR) of a surface can significantly reduce the time to develop coatings used for solar heat management applications. By predicting the TSR, experimental resources are concentrated on the candidates with the best chance of success. Formulations can be tailored to the color requirements, type of substrate, and application parameters.

To allow accurate predictions, the influence of the substrate, pigment composition, pigment percentage, and film thickness must be taken into account by the model. Using properly constructed models to predict the TSR of a surface can point the way to the best coatings solution for specific applications faster using fewer experimental cycles. In the two examples shown, predicted TSR values for the modeled systems agreed with measured values. ❊

References

1. Kubelka, P. and Munk, F., "An Article on Optics of Paint Layers," *Fuer Tekn. Physik, 12*,593-609 (1931).
2. Frey, T., "How to Combine Pigments for Solar-Reflective Colored Coatings," Presented at ABRAFATI, 2011.

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