

Modeling Diffuse Plastic in LightTools

How to Measure Your Plastic or Set Up Mie Particles in Suspension

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Introduction

Diffuse plastics are quite common in illumination applications because they provide an effective way to spatially redistribute light. However, to accurately simulate their performance, you must correctly model the scattering introduced by millions or billions of tiny particles suspended in the base plastic. LightTools illumination and design software supports many methods for modeling diffuse plastics; the hard part is figuring out how to build the model. Typically, you would do one of two things:

- Have samples measured
- Build the material model yourself

This white paper includes a short description of the types of samples that can be measured, as well as a longer walkthrough of the process to build a scattering material model using LightTools software.

Measuring the Scattering Properties of Plastic Materials

Although it can be difficult to do, it is possible to accurately measuring the scattering properties of a plastic. Light Tec (www.lighttec.fr) has a proprietary measurement method that produces data that can be used in LightTools. The measurement requires four samples – typically 1mm, 2mm, 3mm, and 4mm thick. The other dimensions of the samples are commonly at least 25mm in each extent. Each of the faces of the samples should be highly polished to remove (to the extent possible) the possibility of scattering occurring due to surface imperfections. Figure 1 shows a set of acceptable samples provided by Evonik for ACRYLITE Satinice DF23 and by ALBIS for ALCOM PC 740/4 UV CC1063-11LD.

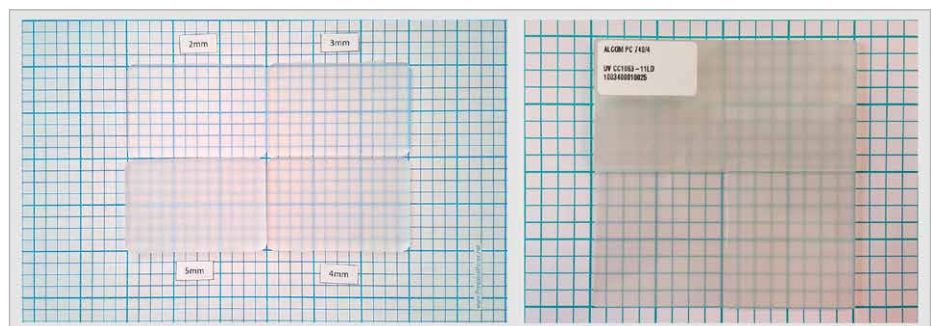


Figure 1: Samples for Evonik ACRYLITE Satinice DF23 (left) and ALBIS ALCOM PC 740/4 UV CC1063-11LD (right) that can be used for scattering measurements

Building a Custom Diffuse Plastic Model in LightTools

Why you would build your own diffuse plastic model instead of having it measured? One example would be if you add particles, such as nano-spheres of titanium dioxide (TiO₂), into a transparent plastic during manufacturing, as opposed to buying and molding a diffuse plastic. A measured model would accurately represent one concentration of particles in the base plastic, but what would happen if you changed the concentration? You would have to re-measure the plastic with the new concentration, and that could be costly and time consuming.

Models for diffuse plastics in LightTools require the definition of three parts: the base plastic, which is sometimes referred to as the “matrix” material, the particles that are in suspension, and the concentration of the particles in the base plastic. We will describe the inputs for each of these in an example that shows how to model an acrylic material with a titanium dioxide pigment.

Defining the Base Plastic

As with every material in LightTools, the definition of your base plastic has two inputs: refractive index and absorption. Ideally, both of these vary as a function of wavelength. If you don't know the specific details about your base plastic, you can use one of the plastics in LightTools' extensive library. The library includes generic plastics, such as polycarbonate or acrylic (PMMA), which offer good starting points, as well as specific materials, such as Evonik ACRYLITE 8N Clear or Covestro Makrolon LED2045, for example.

To begin, choose **Edit > User Materials** from the LightTools main menu, shown in Figure 2.

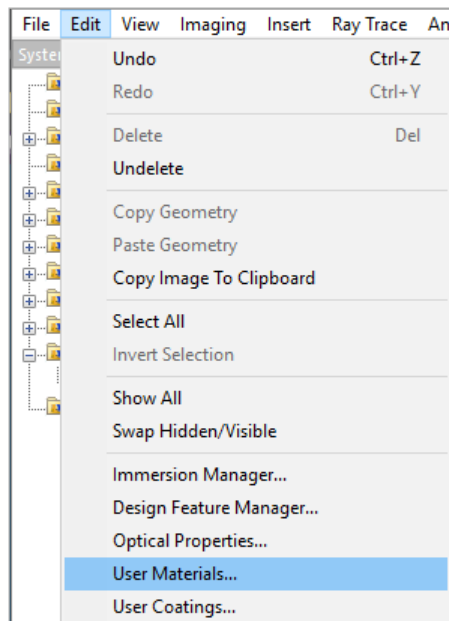


Figure 2: User materials can be defined or edited from the Edit > User Materials menu

This opens the User Material dialog box, which contains the default material “air.” If you intend to use one of the library materials as the base plastic, you can click the Load button and browse to the material file. For this example, we are going to build a plastic from scratch, so click New to create a custom material. You can change the name of the plastic; in this case, we chose “DiffusePlastic,” as shown in Figure 3.

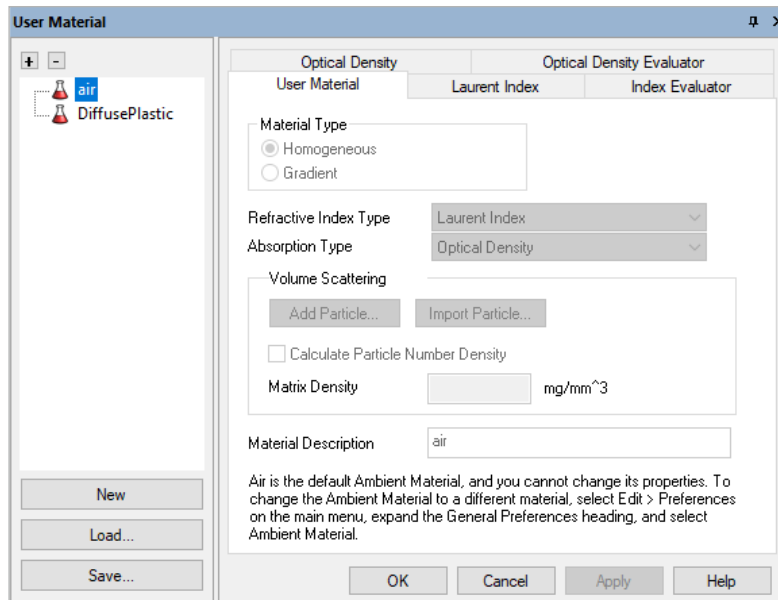


Figure 3: The User Material dialog box after a new material has been added

Select the new plastic in the navigation tree on the left, and the inputs required for it are displayed in the tabs on the right.

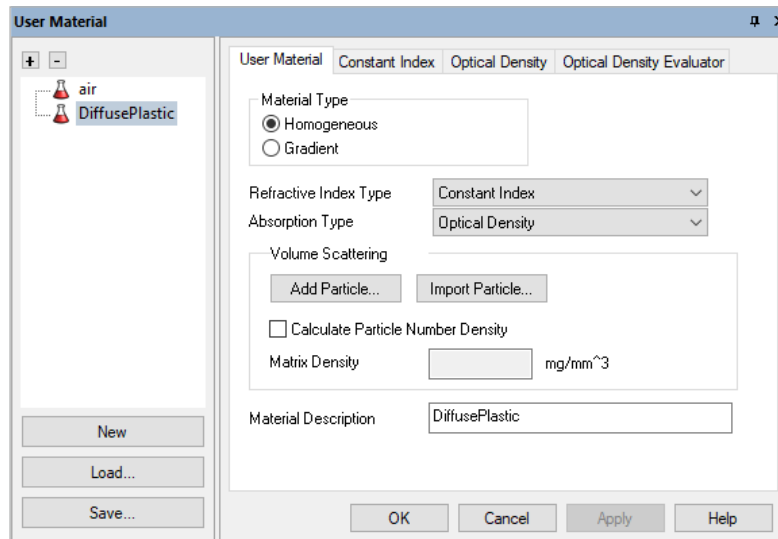


Figure 4: The initial state of the DiffusePlastic material

The Material Type for our plastic is homogeneous, and we will be specifying the refractive index and the absorption. LightTools supports several models for each of these inputs. The next two sections describe the models and inputs required for each of them.

Models for Refractive Index and Dispersion

LightTools has eight built-in models for specifying a material's index of refraction. The inputs required for these are shown in Table 1, below. With the exception of Index Interpolation, all formulae and their coefficients assume that the wavelength of light is given in microns.

Name	Formula
Constant	$n(\lambda) = A$
Index Interpolation	Set of wavelength-index pairs: 450nm, 1.625 550nm, 1.586 650nm, 1.525 750nm, 1.487 ...
Cauchy	$n(\lambda) = A_0 + \frac{A_1}{\lambda^2} + \frac{A_2}{\lambda^4}$
Hartmann	$n(\lambda) = A_0 + \frac{A_1}{(A_2 - \lambda)^{1.2}}$
Sellmeier	$n^2(\lambda) = 1 + \frac{B_1\lambda^2}{\lambda^2 - C_1^2} + \frac{B_2\lambda^2}{\lambda^2 - C_2^2} + \frac{B_3\lambda^2}{\lambda^2 - C_3^2} + \frac{B_4\lambda^2}{\lambda^2 - C_4^2} + \frac{B_5\lambda^2}{\lambda^2 - C_5^2} + \frac{B_6\lambda^2}{\lambda^2 - C_6^2}$
Glass Manufacturer's Sellmeier	$n^2(\lambda) = 1 + \frac{B_1\lambda^2}{\lambda^2 - C_1} + \frac{B_2\lambda^2}{\lambda^2 - C_2} + \frac{B_3\lambda^2}{\lambda^2 - C_3} + \frac{B_4\lambda^2}{\lambda^2 - C_4} + \frac{B_5\lambda^2}{\lambda^2 - C_5} + \frac{B_6\lambda^2}{\lambda^2 - C_6}$
Laurent	$n^2(\lambda) = A_0 + A_1\lambda^2 + \frac{A_2}{\lambda^2} + \frac{A_3}{\lambda^4} + \frac{A_4}{\lambda^6} + \frac{A_5}{\lambda^8}$
Glass Manufacturer's Laurent	$n^2(\lambda) = A_0 + A_1\lambda^2 + \frac{A_2}{\lambda^2} + \frac{A_3}{\lambda^4} + \frac{A_4}{\lambda^6} + \frac{A_5}{\lambda^8} + A_6\lambda^4 + \frac{A_7}{\lambda^{10}} + \frac{A_8}{\lambda^{12}}$

Table 1: Dispersion Models in LightTools

Models for Absorption

LightTools provides five ways to enter absorption data, all of which follow the Beer-Lambert law. Table 2 summarizes each of the types and shows their relationship to the wavelength dependent internal transmittance of the material, $T_i(\lambda)$, at a specific thickness of the material, L , in millimeters. All quantities are unitless except Optical Density, whose unit is 1/mm.

Name	Symbol	Formula	Inputs
Transmittance/Length	$T_i(\lambda)$		Set of wavelength-transmittance pairs and the length (L): 450nm, 0.9568 550nm, 0.9684 650nm, 0.9654 750nm, 0.8651 ...
Constant Transmittance/Length		$T_i(\lambda) = A$	Singular internal transmittance value and the length
Optical Density	$D(\lambda)$	$D(\lambda) = \frac{\log_{10} \frac{1}{T_i(\lambda)}}{L}$	Set of wavelength-density pairs: 450nm, 1.625E-3 550nm, 1.586E-3 650nm, 1.525E-3 750nm, 1.487E-3 ...
Constant Optical Density		$D(\lambda) = B$	Singular optical density value
Extinction Coefficient	$k(\lambda)$	$T_i(\lambda) = e^{-\frac{4\pi k(\lambda)L}{\lambda}}$	Set of wavelength-coefficient pairs: 450nm, 1.258E-5 550nm, 1.586E-5 650nm, 1.525E-5 750nm, 1.487E-5 ...

Table 2: Absorption Models in LightTools

The Complete Base Plastic Model

Obtaining good optical data for plastics can be difficult. For our example, we will use refractive index data for PMMA that is available on RefractiveIndex.Info (www.refractiveindex.info). One of the references (Szczurowski 2013) has refractive index data from 405nm to 1080nm using Glass Manufacturer's Sellmeier coefficients, shown in the equation below.

$$n^2(\lambda) = 1 + \frac{0.99654\lambda^2}{\lambda^2 - 0.00787} + \frac{0.18964\lambda^2}{\lambda^2 - 0.02191} + \frac{0.00411\lambda^2}{\lambda^2 - 3.85727}$$

In the User Material dialog box, with DiffusePlastic selected, choose GM Sellmeier for the Refractive Index Type, shown in Figure 5, and click Apply.

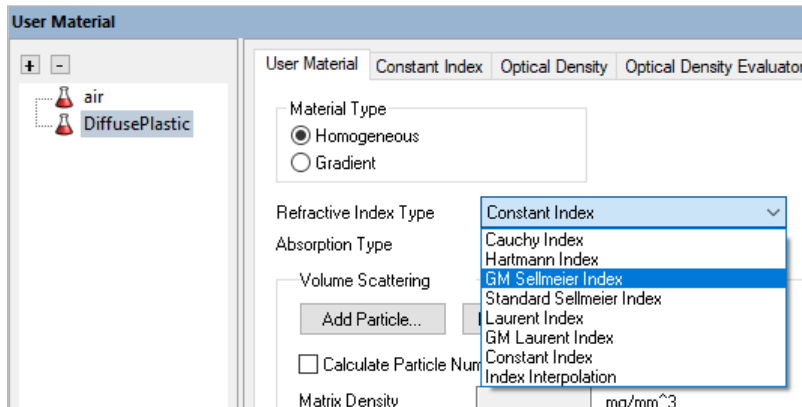


Figure 5: Refractive index types available for homogeneous materials

On the resulting GM Sellmeier Index tab, enter the coefficients in the equation as shown in Figure 6.

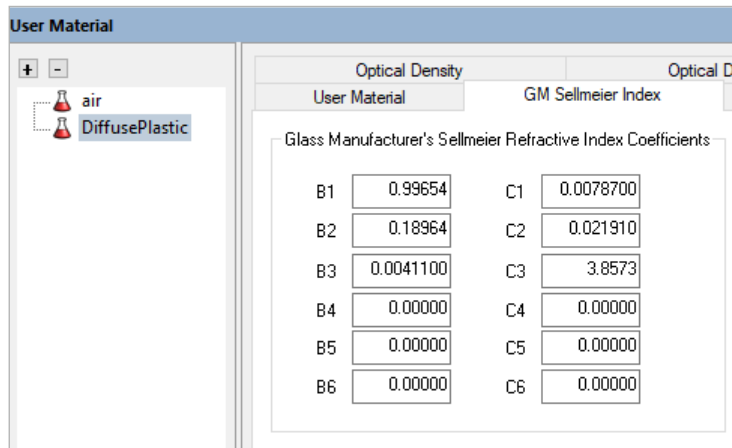


Figure 6: The Glass-Manufacturer's Sellmeier coefficients as entered from the Szczurowski 2013 data

After you enter the data, it's a good idea to check the Index Evaluator to verify that the values are reasonable. Click the Index Evaluator tab. Figure 7 shows that the index at 550nm is 1.4924, using the entered coefficients, which is about what we expect.

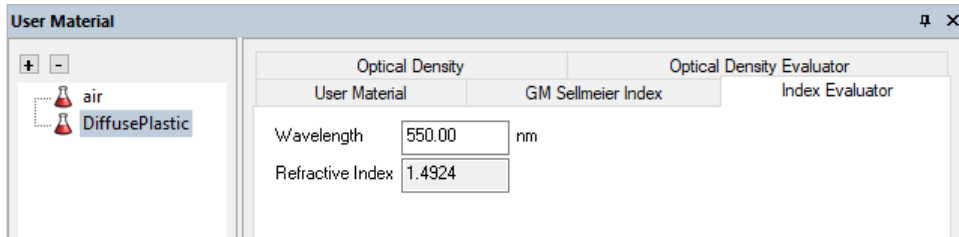


Figure 7: The Index Evaluator allows you to verify the refractive index that is calculated for any given wavelength

Absorption data can be even more difficult to find for the generic case. The Handbook of Plastic Optics, edited by Stefan Bäumer, shows that the internal transmittance of PMMA is about 0.9 across the visible spectrum for a 3mm thickness. Although it would be better to have data that varies with wavelength, we can use this as a rough estimate. On the User Material tab, change the Absorption Type to Constant Transmittance/Length, shown in Figure 8, and click Apply.

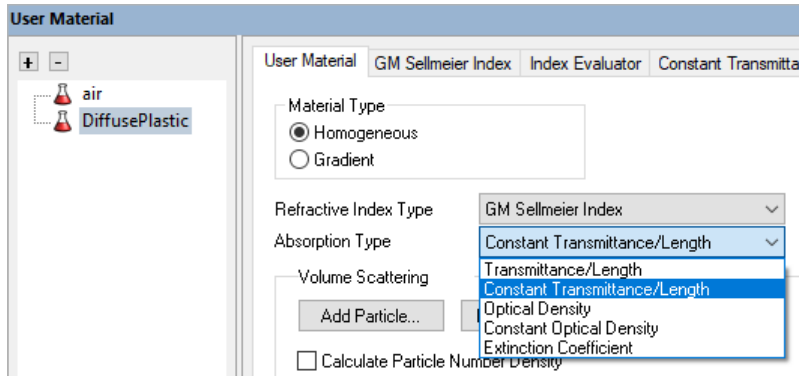


Figure 8: The list of absorption types that are available in LightTools

On the Constant Transmittance/Length tab, shown in Figure 9, enter 0.9 for the transmittance and 3mm for the length and click Apply.

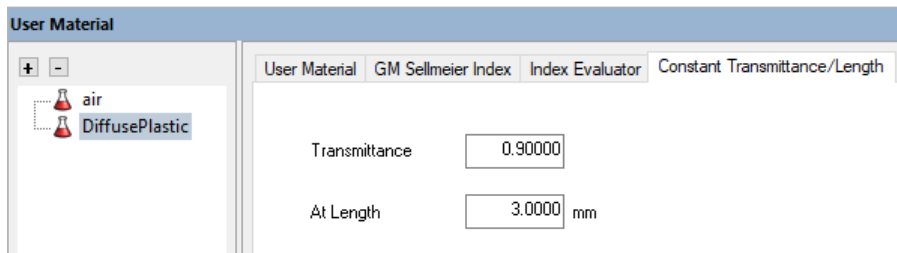


Figure 9: The Constant Transmittance/Length data as entered

The model for the base plastic is now complete.

Defining the Particles in Suspension

In the real world, to make a diffuse plastic, we would mix a quantity of small particles into a plastic as it's being molded. In LightTools, we do the same thing. We start with the base plastic and add particles in suspension. On the User Material tab for DiffusePlastic, click the Add Particle button to see a list of available particles and select Mie, as shown in Figure 10.

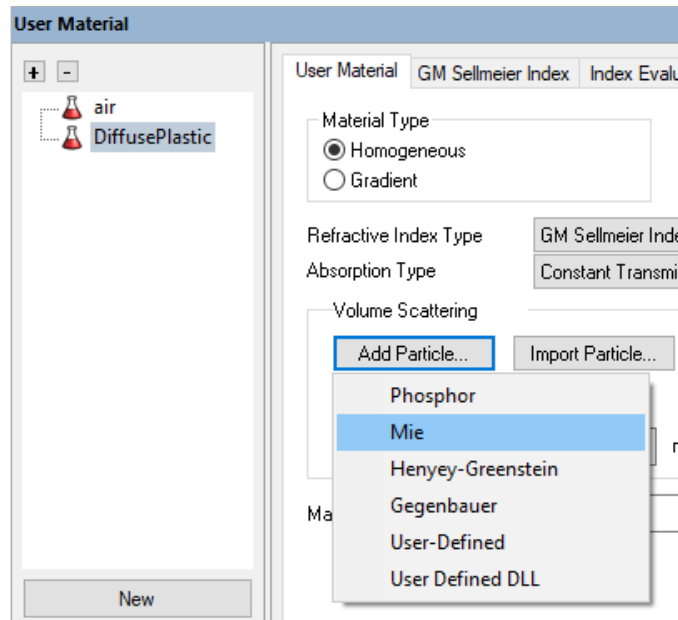


Figure 10: The list of available particle types

Of the available particle options, phosphors are a special case. When light strikes a phosphor particle, the light can be absorbed and re-emitted as light of a different wavelength. Of the remaining particle types, Mie, Henyey-Greenstien, Gegenbauer, and User-Defined, only the Mie model allows you to enter physical parameters about the particles themselves, as we will see. The other particles allow you to directly enter or change, via formula coefficients, the direction that light scatters after it interacts with a particle. Since we are making our own diffuse plastic and know more about the physical properties of the particles than the scattering properties, the Mie option is the best choice.

In the navigation tree on the left, our DiffusePlastic now has a sub-node labeled Mie1, shown in Figure 11.

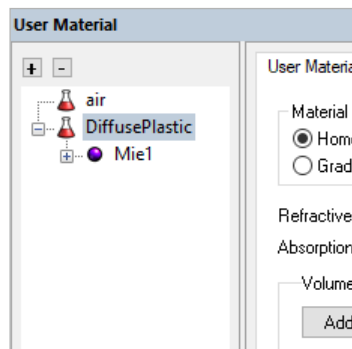


Figure 11: After adding a Mie particle to the DiffusePlastic material, a new node is shown in the navigation tree

Select the Mie1 sub-node to see tabs for Controls and Mie Particle Size, shown in Figure 12. We will modify parameters on both of these tabs.

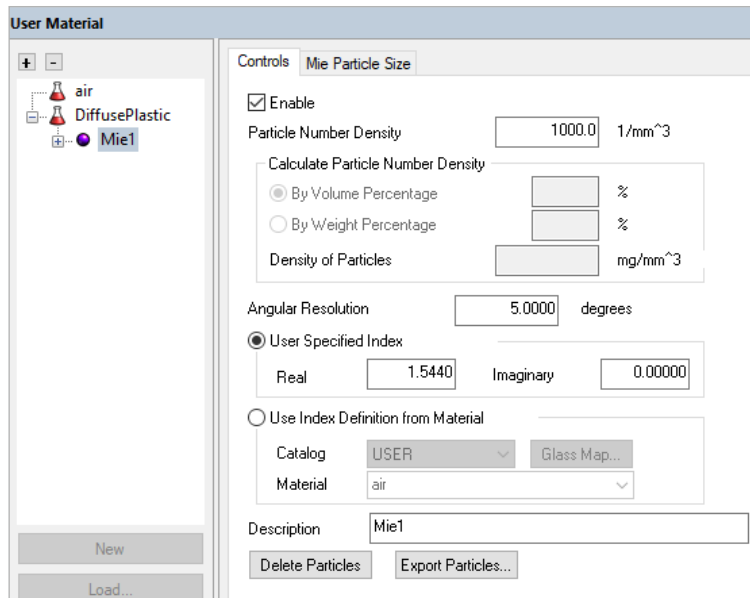


Figure 12: The available controls for a Mie particle

On the Controls tab, we need to specify the optical properties of the particles. You can do this using one of two options shown in Figure 13: by specifying the real and imaginary index of refraction or by choosing an existing material. The User Specified Index option is useful if you know the refractive index and extinction coefficient at only one wavelength. This option is better than nothing; however, as previously stated, using data that varies with wavelength is preferable.

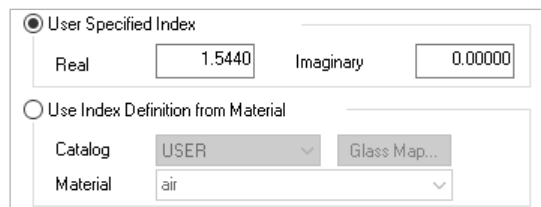


Figure 13: Material properties for the particles can be specified by entering the refractive index or by selecting an existing material

To use a material from the catalog, we first need to create it. Let's assume we want the particles in suspension to be nano-spheres of titanium dioxide (TiO₂). RefractiveIndex.Info has data published for TiO₂ as a thin film that should be adequate for this example. In the User Material dialog box, click New to create a new User Material and name it TiO₂, as shown in Figure 14.

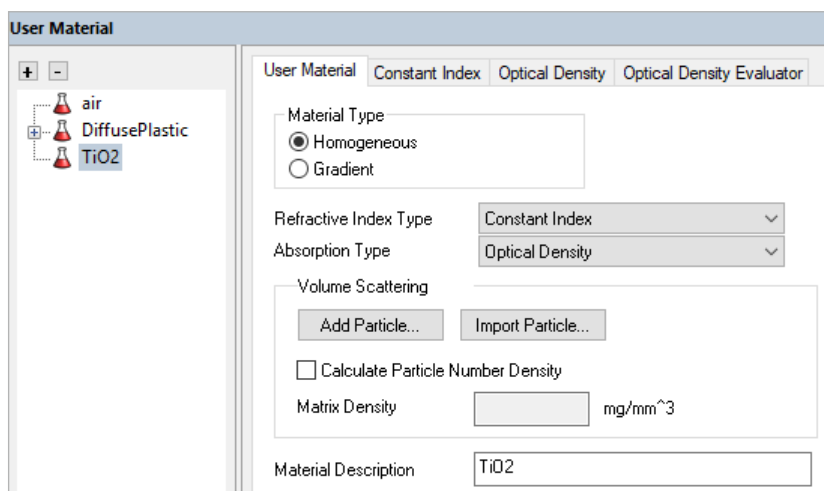


Figure 14: A new material has been created for TiO2

The Siefke et al. 2016 data for n and k is tabular in both instances. For these, we choose Index Interpolation for the Refractive Index Type and Extinction Coefficient for the Absorption Type. The wavelength data from the website is in microns, so it must be converted to nanometers to use in LightTools. Realistically, we need only the visible portion of each dataset, so we can truncate this long dataset. After copying and pasting the data into the correct tabs in LightTools, you should get a refractive index of 2.4358 at 550nm and an extinction coefficient of 5.3945e-8 at 550nm when reviewing the Index Evaluator tab and the Extinction Coefficient Evaluator tabs, respectively.

Now, going back at the Mie particle of the DiffusePlastic, you can choose Use Index Definition from Material on the Controls tab, set the catalog to USER, and select TiO2 from the list of available materials, as shown in Figure 15.

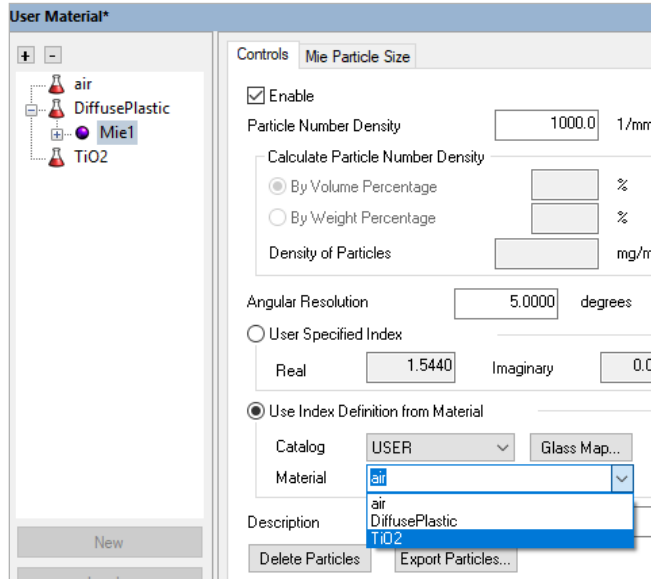


Figure 15: Once the particle's material has been created, it can be selected from the USER catalog

Finally, we need to define the particle size distribution for the TiO2 particles. You can use a single size, but, as with everything else, a more realistic distribution provides better results. In many cases, manufacturers provide particle size distribution as a median and standard deviation. As an example, The Chemours Company recommends their Ti-Pure R-104 as a TiO2 powder for injection molded plastics. The datasheet shows a mean particle size of 220nm, but provides no standard deviation. The full-width at half maximum can be approximated from a curve on a different datasheet to be 150nm, which is a standard deviation of 64nm. We will use those parameters for this example. You can use a spreadsheet (e.g., Excel) to create a simple normal distribution whose mean (μ) is 220nm and whose standard deviation (σ) is 64nm using the following equation.

$$f(x) = e^{-\frac{(x-\mu)^2}{2\sigma^2}} = e^{-\frac{(x-220)^2}{2 \cdot 64^2}}$$

Figure 16 shows the particle size distribution that we entered. A weight ($f(x)$ from the equation above) was entered every 5nm from 5nm to 435nm. You could use fewer data points, if desired.

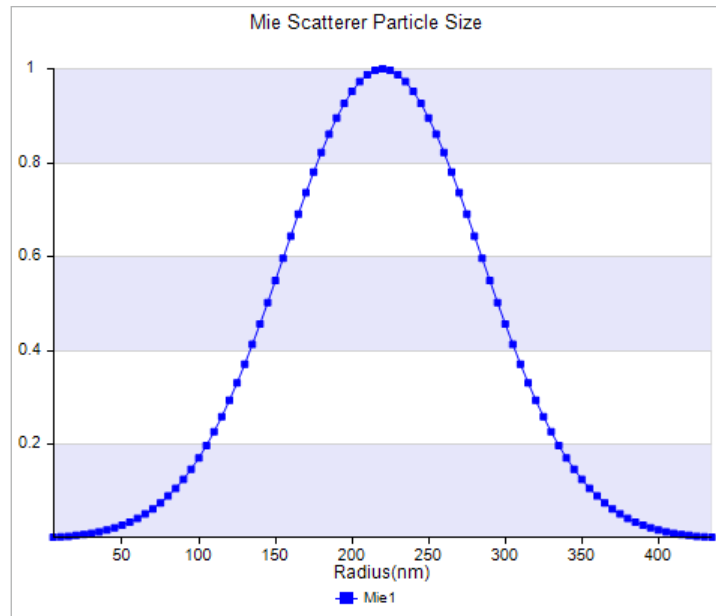


Figure 16: The particle size distribution as input into LightTools

Defining the Concentration of Particles

The final input to the material model is the number of particles in the base plastic. There are three ways to define the concentration:

- Input the number of particles directly.
- Input the fraction of the volume occupied by the particles vs. the base plastic.
- Input the fraction of the weight occupied by the particles vs. the base plastic.

Specifying the Number of Particles

The simplest way to specify the concentration of particles is to input the number of particles per cubic millimeter. This is specified as the Particle Number Density on the Controls tab of the Mie particle, shown in Figure 17. This number can easily be in the millions or billions.

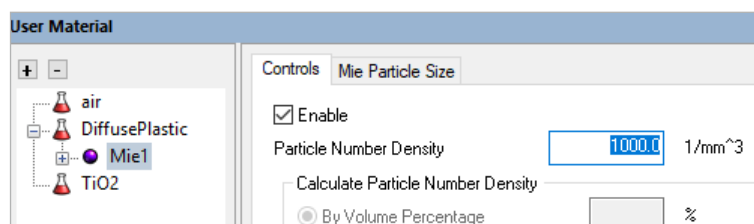


Figure 17: The Particle Number Density specifies the number of particles per cubic millimeter

Specifying the Volume Fraction or Weight Fraction

The other two input methods are very similar to each other. You can specify either the percentage of the combined volume occupied by the particles or the percentage of the combined weight occupied by the particles. Both of these are measurable and may be the best for the data that we have. For example, we could weigh how much base plastic that we're using (W_b), and we could weigh the particles that we put into that amount of base plastic (W_p) and then calculate the By Weight Percentage of the particles ($\%_W$) using the following equation.

$$\%_W = \frac{W_p}{W_b + W_p} \cdot 100\%$$

The By Volume Percentage can be calculated using a similar formula.

To use either of these two inputs, you must know the density of both the base plastic and the particles. For our example, a quick internet search reveals the density for PMMA as 1.18 g/cm³ and the density for titanium dioxide as 4.23 g/cm³. The base plastic's density is input on the User Material tab of the DiffusePlastic. You must enable the Calculate Particle Number Density option and enter the density as mg/mm³, which is the same as g/cm³, as shown in Figure 18. Click Apply.

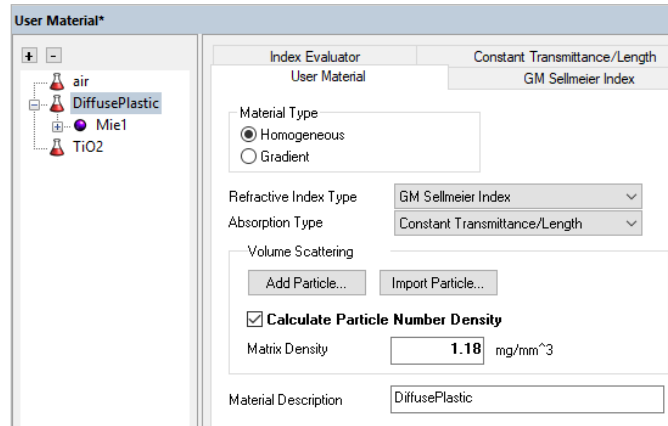


Figure 18: The density of the base material is entered on the User Material tab

Next, you need to enter the particle density on the Controls tab of the Mie particle as shown in Figure 19. Click Apply.

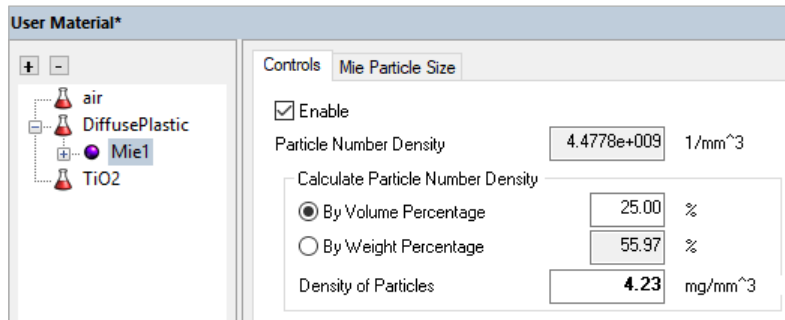


Figure 19: The density of the particles is entered on the Controls tab of the particle

Finally, choose By Volume Percentage or By Weight Percentage and enter the desired concentration, as shown in Figure 20. After clicking Apply, your material is completely defined and ready to use for simulation.

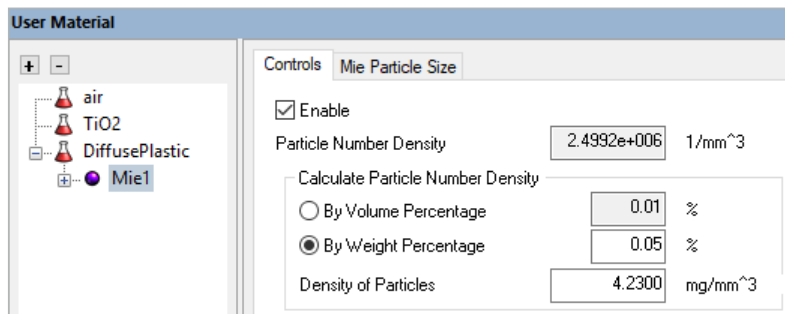


Figure 20: The concentration of the particles in this example is entered as a By Weight Percentage of 0.05%

Validating the Diffuse Plastic Model

Checking to make sure that your material model is correct can be tricky. The Mie Evaluator, which is available as a sub-node of the Mie particle, can provide some insight. Using our example model, Figure 21 shows that the Mean Free Path of the diffuse plastic is 0.73mm. This means that, on average, a ray would propagate through 0.73mm of base plastic before hitting a TiO₂ particle. If the light is traveling through 0.75mm of material, then half of the rays would strike a particle, and the other half would not. Traveling through more material means that the light is more likely to be scattered.

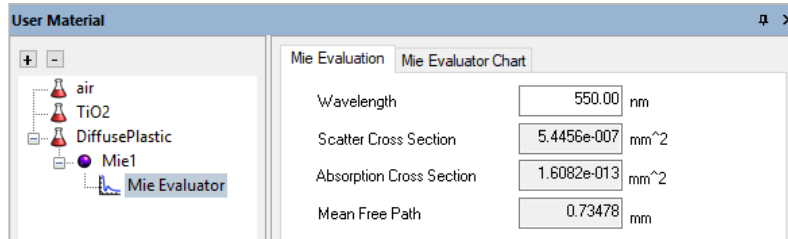


Figure 21: The Mie Evaluator shows metrics that are calculated based on the other inputs

Perhaps the best method of validating the material setup is to trace some rays and verify that the result is reasonable. Figure 22 shows LightTools simulation results for three concentrations of TiO₂. Each case is a rendering of a sample plaque with four different thicknesses as it sits above a blue and white sheet of graph paper. The images show, from left to right, a 0.05% By Weight concentration, a 0.1% By Weight concentration, and a 1% By Weight concentration. These concentrations correspond to 0.75lbs, 1.5lbs, and 15.2lbs of TiO₂ per 1500lb gaylord of PMMA, respectively.

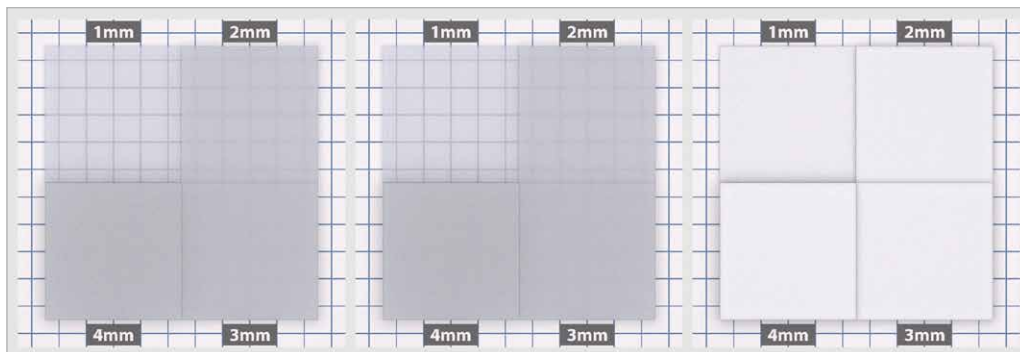


Figure 22: LightTools renderings of a four-thickness sample plaque with three different by-weight concentrations of TiO₂: 0.05%, 0.1%, and 1.0%, from left to right