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.

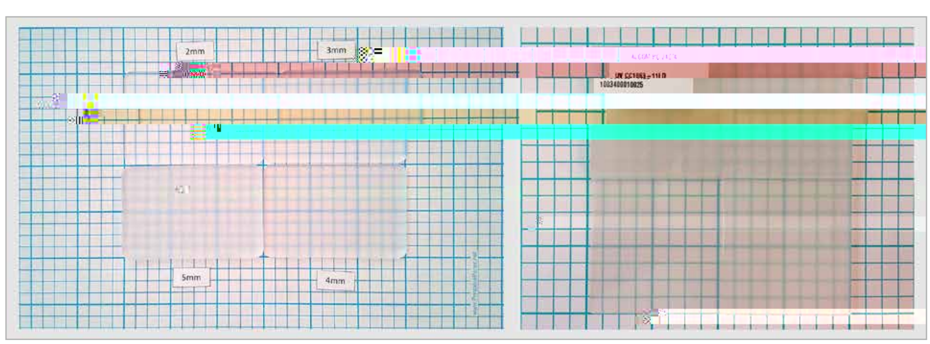


Figure 1: Samples for Evonik ACRYLITE Satinice DF23 (left) and ALBIS ALCOM PC 744/4 UV CC1063-11LD (right) that can be used for scattering measurements

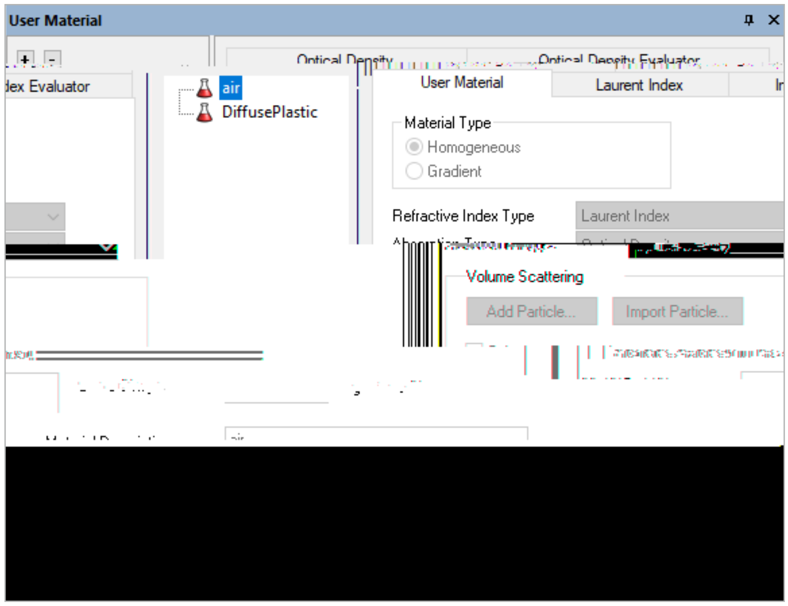


Figure 3: The User Material dialog box after a new material has been added

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.

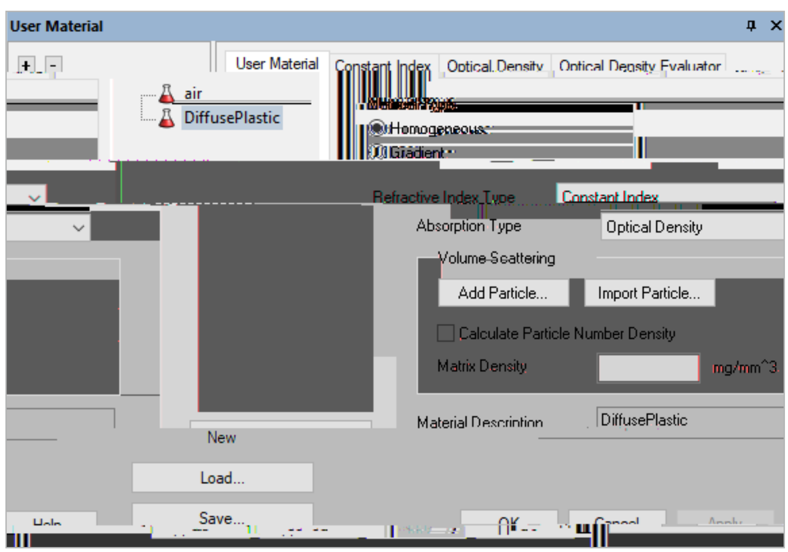


Figure 4: The initial state of the DiffusePlastic material

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	
Index Interpolation	Set of wavelength-index pairs:
Cauchy	
Hartmann	
Sellmeier	
Glass Manufacturer’s Sellmeier	

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.

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

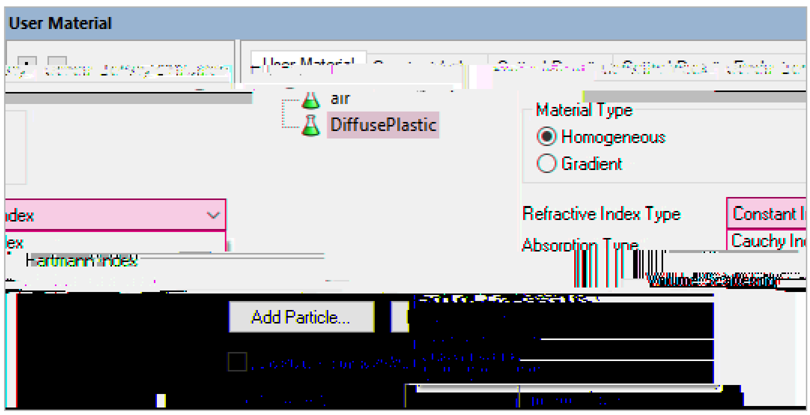


Figure 5: Refractive index types available for homogeneous materials

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

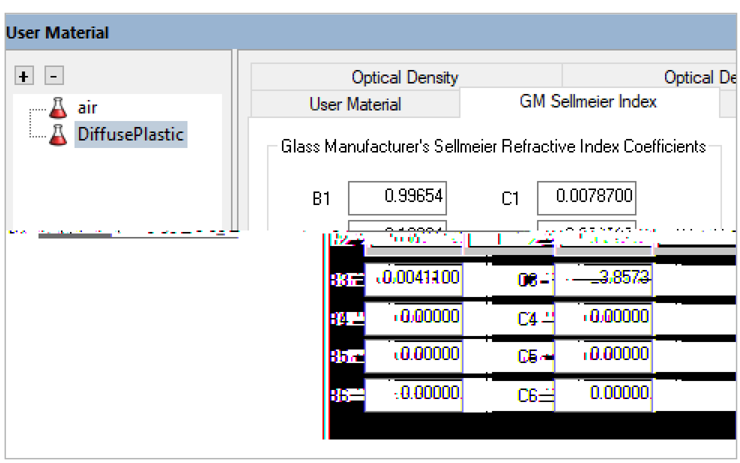


Figure 6: The Glass-Manufacturer's Sellmeier coefficients as entered from the Szczurowski 2013 data

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.

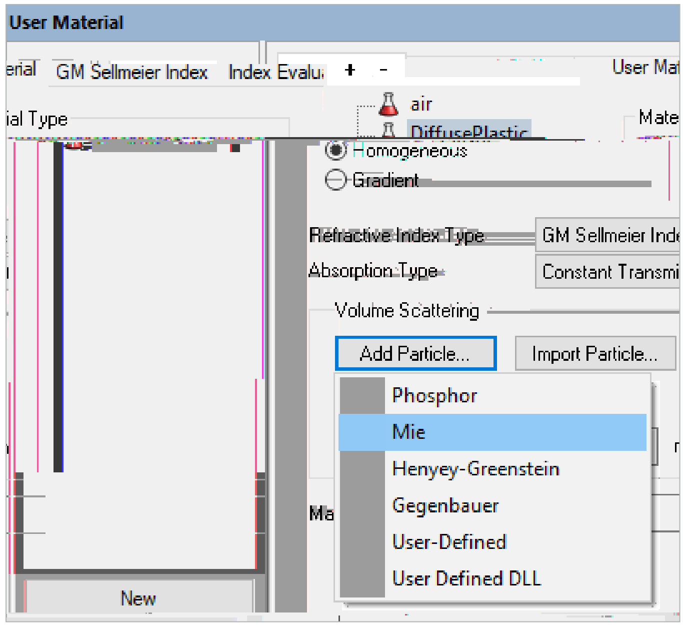


Figure 10: The list of available particle types

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,

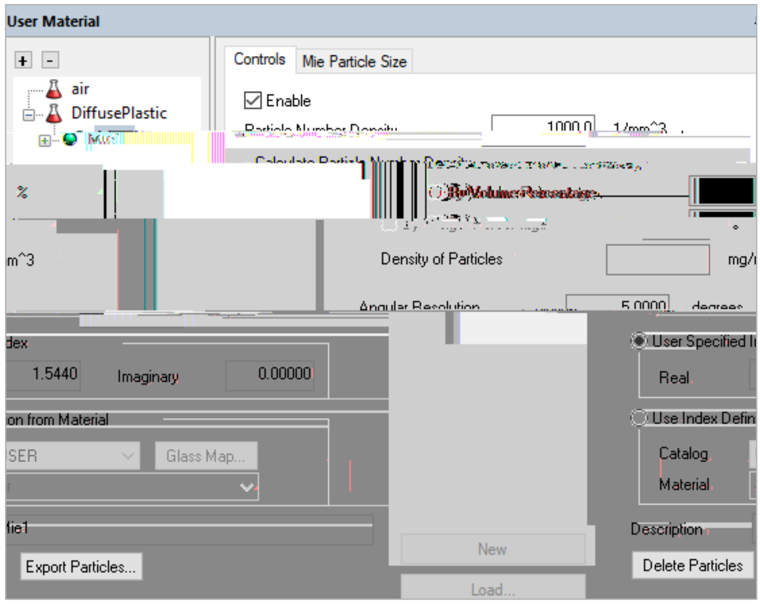


Figure 12: The available controls for a Mie particle

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.

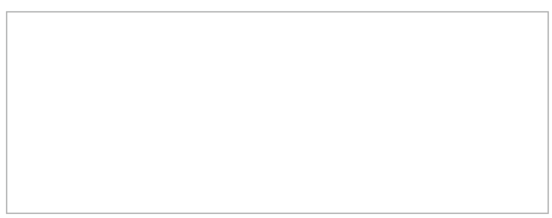


Figure 13: Material properties for the particles can be specified by entering the refractive index or by selecting an existing material

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.

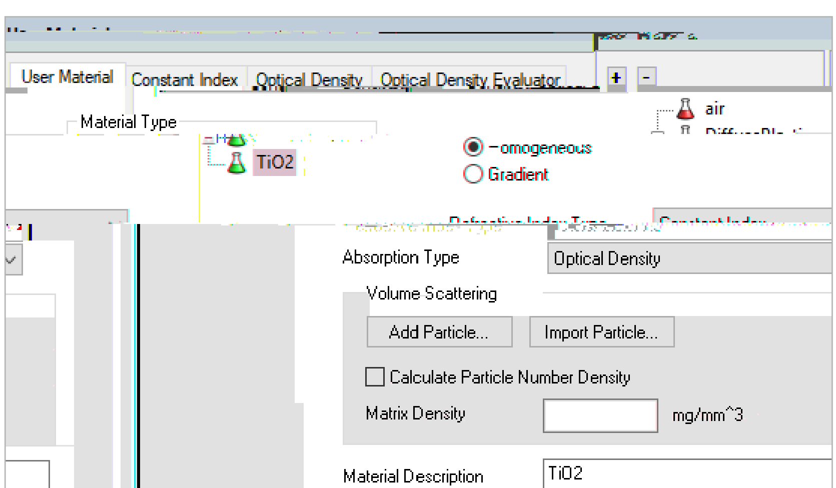


Figure 14: A new material has been created for TiO2

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.

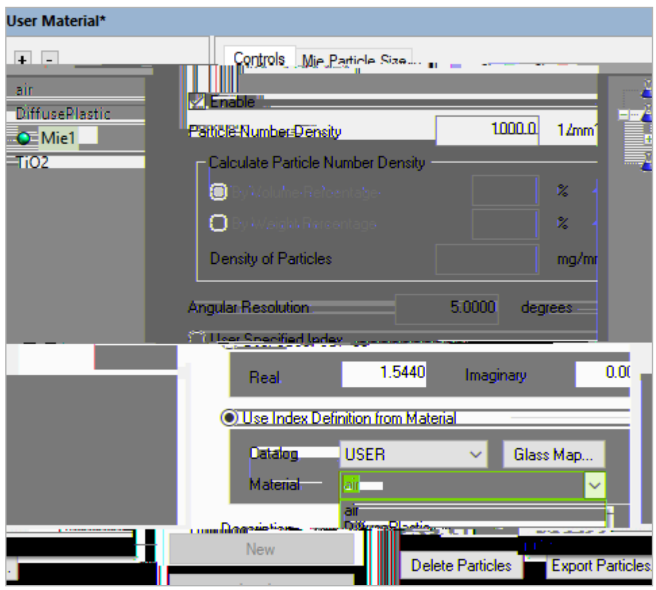
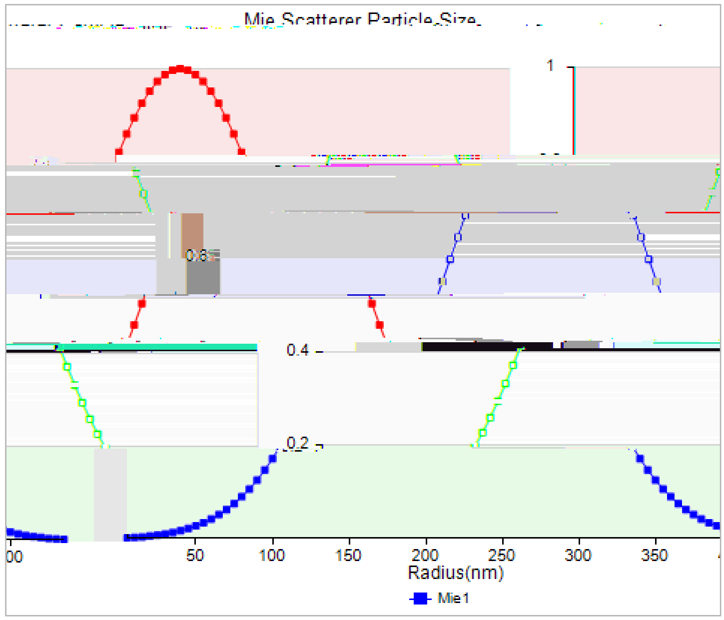


Figure 15: Once the particle's material has been created, it can be selected from the USER catalog

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 RCTCOGVGTU HQT VJKU GZCORNG ;QW ECP WUG C URTGCFUJGGV G I 'ZEGN VQ CPF YJQUG UVCPFCTF FGXKCVKQP Ä KU PO WUKPI VJG HQNNQYKPI GSWCVKQP

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.



Mie Scatterer Particle Size
1
0.8
0.4
0.2
00
50
100
150
200
250
300
350
Radius(nm)
Mie1

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.

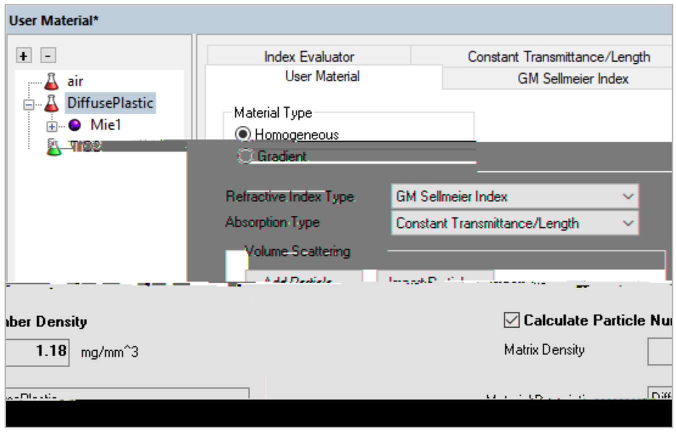


Figure 18: The density of the base material is entered on the User Material tab

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

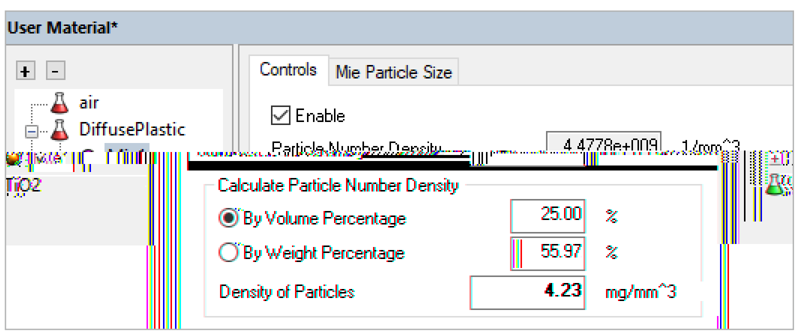


Figure 19: The density of the particles is entered on the Controls tab of the particle

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.

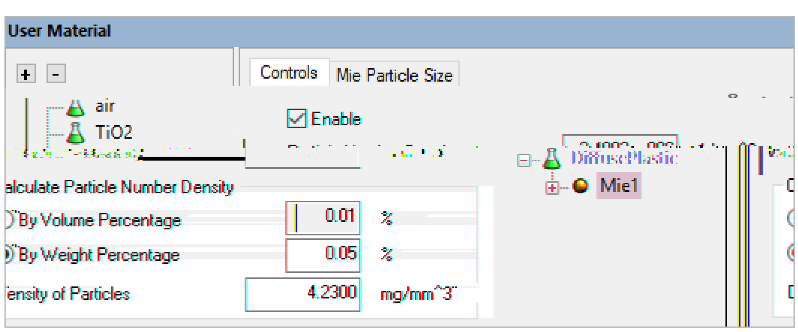
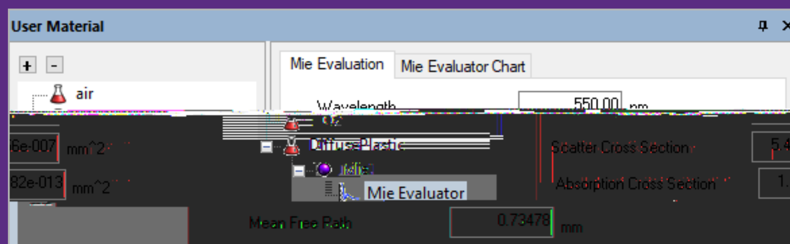


Figure 20: The concentration of the particles in this example is entered as a By Weight Percentage of 0.05%

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.



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