

Phosphors exhibit photoluminescence, the process by which a material absorbs light of a specific spectral range and re-emits light of another spectral range with longer wavelengths. Because of the increased availability of phosphor-based white light-emitting diodes, the use of phosphors is increasingly prevalent in illumination design. To ensure that simulations for such illumination designs are accurate, it is important to accurately model the optical effects of phosphors. To describe how phosphors are modeled in *LightTools*, this paper explains how *LightTools* inputs correlate to theoretical models, as well as how to obtain the necessary data.

## Phosphor 101

The law of conservation of energy states that when light is absorbed by a material, the energy must go somewhere. In most materials, the energy is converted to heat; however, in photoluminescent materials part of the energy is converted to heat, while the rest is converted to longer wavelength light. One way to visualize this concept is to consider an electron band diagram, as shown in Figure 1.

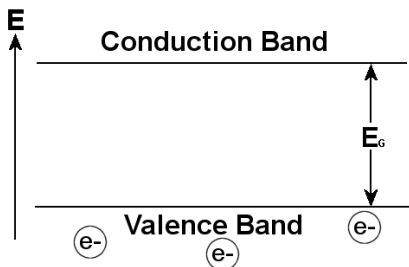


Figure 1. Electron band diagram

Electrons orbiting an atom's nucleus have discrete energy levels, and a similar energy structure exists in many materials. However, instead of the discrete energy levels found in atoms, the molec-

ular structure results in energy bands for the electrons. The *valence band*, a lower, steady-state energy level, is represented in Figure 1 as the baseline. The *conduction band*, the higher energy state at which electrons are free to flow in the material, is represented as the higher level in the diagram. The vertical axis of the chart represents the energy level, with higher energy levels toward the top of the chart.

The distance between the two energy levels,  $E_G$ , known as the *bandgap energy*, is determined by the atomic configuration of the material. Phosphor designers typically add impurities to a phosphor crystal (a practice known as "doping") to adjust the bandgap to accept and emit particular wavelengths of light.

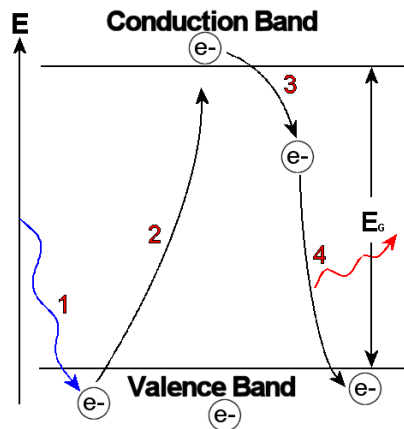


Figure 2. The process of photoluminescence

Figure 2 shows, in simplified terms, the process of photoluminescence. In step 1, a photon of light is absorbed by the material. If the photon energy is equal to  $E_G$ , an electron in the valence band jumps the bandgap to the conduction band, as shown in step 2. The energy of

the input photon,  $E_{in}$ , is known from the wavelength of light and Equation (1).

$$E = \frac{hc}{\lambda} \quad (1)$$

where

$h$  = Planck's Constant

$c$  = speed of light

$\lambda$  = wavelength

In reality, there are many sub-excited states that occur just above or below the conduction band. These extra states allow a material to accept a photon whose energy is not exactly equal to the bandgap energy. The set of wavelengths that are absorbed by the material define the *absorption spectrum* for the phosphor.

After a time, the excited electron will return to its base state - an event that is accompanied by a release of energy. If the material releases this energy over a long period of time, usually measured in minutes or hours, the material is said to be *phosphorescent*. If the energy is released almost instantaneously, then the material is called *fluorescent*. The phosphors used in illumination systems are typically fluorescent. For the purpose of this paper, materials that exhibit fluorescence or materials that contain particles that exhibit fluorescence are called phosphors.

In most cases, the electron does not fall directly from the excited state to the base state. Instead, it falls to any number of sub-excited states before returning to the base state, as shown in step 3 and step 4 of Figure 2. The energy released from the smaller transitions is realized only as heat, while the larger transitions can release photons in the visible range. However, since the amount of energy released in step 4 is less than the energy of the absorbed photon, the wavelength

emitted is always longer than that of the absorbed photon. The difference between the absorbed and emitted photon energy is commonly known as the Stoke's Shift. In reality, there are other non-radiative losses that occur in the crystal.

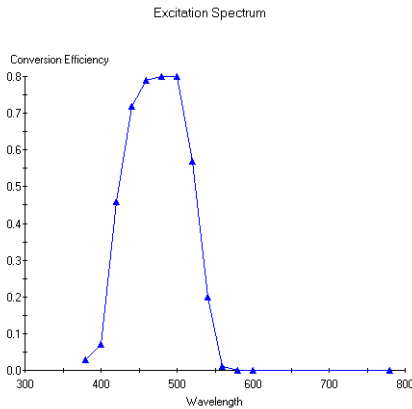
Based upon the preceding description of the interactions between a photon and the phosphor, it is possible to formulate energy balance equations for a phosphor. In order to conserve energy in the phosphor, Equation (2) must be true.

$$E_{in} = E_{out} \quad (2)$$

The output energy can be broken into two parts: the energy that is absorbed by the material, and the energy that passes through the material or is scattered without being absorbed. The absorbed energy,  $E_{\alpha}$ , is dictated by the absorption spectrum.

$$E_{in} = E_{unabsorbed} + E_{\alpha} \quad (3)$$

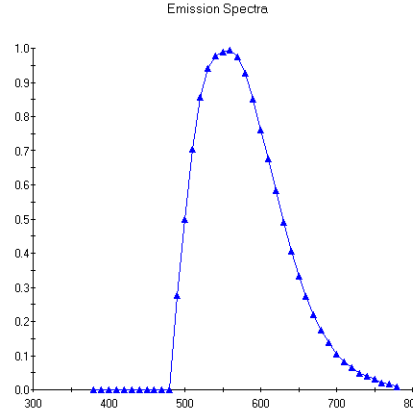
Not all of the energy absorbed by the phosphor is re-emitted as light. The set of wavelengths absorbed by the phosphor that cause light to be re-emitted is known as the *excitation spectrum*. The set of wavelengths that define the excitation spectrum is a proper subset of the wavelengths that define the absorption spectrum. Figure 3 shows an the excitation spectrum for the default phosphor material in *LightTools*.



**Figure 3. Default *LightTools* excitation spectrum**

The wavelength of the emitted light energy is longer than the wavelength of

the absorbed light, and those wavelengths of light that are emitted from the phosphor define the *emission spectrum*. The emission spectrum is a function of the wavelength of the absorbed light, but generally doesn't vary much. The emission spectrum for the default phosphor in *LightTools* is shown in Figure 4.



**Figure 4. Default *LightTools* emission spectrum**

The absorbed energy not converted into the emission spectrum is released as heat or through some other non-radiative transfer. The heat energy represents the Stoke's Shift, shown as  $E_{SS}$ , and the non-radiated energy,  $E_{nonRad}$ , as shown in Equation (4).

$$E_{\alpha} = E_{SS} + E_{converted} + E_{nonRad} \quad (4)$$

When Equation (3) and Equation (4) are combined, the full energy balance equation, shown in Equation (5), is obtained.

$$E_{in} = E_{unabsorbed} + E_{SS} + E_{converted} + E_{nonRad} \quad (5)$$

The simulations performed in *LightTools* accurately depict the state of energy for a single moment in time. Because energy can vary with time, the formulas in this paper replace energy (E) with power ( $\Phi$ ), a time invariant quantity defined, in this case, as the light energy per unit time. With this distinction in mind, Equation (5) becomes:

$$\Phi_{in} = \Phi_{unabsorbed} + \Phi_{SS} + \Phi_{converted} + \Phi_{nonRad} \quad (6)$$

## Phosphors in *LightTools*

*LightTools* provides the ability to model phosphors as user-defined materials with phosphor particles in suspension. It is important to note that to create or use a phosphor material in *LightTools*, you must have access to the Advanced Physics Module. If you do not currently have the Advanced Physics Module, contact ORA at support@opticalres.com for licensing information.

Many inputs are required to accurately model a phosphor in *LightTools*. To understand the need for each of the inputs, first consider the energy balance that occurs during the ray trace. In *LightTools*, a ray propagates through the material until it leaves the material or strikes a phosphor particle. Because *LightTools* models light stochastically, the power balance for each ray that strikes a phosphor particle is defined using probabilities and percentages.

## Ray Trace Power Balance

Consider a ray with power  $\Phi_0$  and wavelength  $\lambda_0$  that enters a phosphor material. The average distance the ray travels without hitting a phosphor particle is determined by the *mean free path* between the phosphor particles. *LightTools* also allows the material to contain non-luminescent, or inert, particles, that have their own mean free path. The probability that the ray will hit an inert particle instead of a phosphor particle is calculated automatically. If the ray strikes an inert particle, it is scattered according to the inert particle's scattered intensity function.

If the ray strikes the phosphor particle, *LightTools* first determines if the ray is absorbed. This is determined from the absorption spectrum,  $\alpha(\lambda)$ . Unlike other absorption spectra in *LightTools*, the absorption spectrum for a phosphor particle does not necessarily imply loss of power. Using the electron band diagram analogy from earlier, the absorption spectrum for a phosphor determines only whether or not a ray has the correct wavelength to cause an electron to jump the bandgap. It is possible that all of the absorbed energy is dissipated without light emission. It is also possible that the

power of the ray will be re-emitted, which is determined by the excitation spectrum or quantum yield, defined in “Excitation Spectrum/Quantum Yield” on page 5. If the ray is not absorbed ( $\alpha(\lambda_0) = 0$ ), it propagates away from the particle as defined by the intensity distribution for unconverted rays, described in “Unconverted Intensity” on page 6.

The remainder of the energy balance changes depending on whether or not an excitation spectrum or quantum yield is used. When an excitation spectrum is used, *LightTools* assumes that the effect of Stoke’s shift is included in the excitation spectrum. When quantum yield is used, *LightTools* dynamically calculates the loss due to Stoke’s Shift.

### Power Balance using an Excitation Spectrum

If the ray is absorbed, *LightTools* determines from the excitation spectrum ( $Ex(\lambda)$ ) whether or not a ray is re-emitted from the particle. If the ray is not re-emitted, ( $Ex(\lambda_0) = 0$ ), it stops at the particle, and the power ( $\Phi_0$ ) is lost. If a ray is re-emitted, the total power,  $\Phi_{Em}$ , in the emission spectrum,  $Em_{\lambda_0}(\lambda)$ , for the incident wavelength is the power remaining from the incident ray, as shown in Equation (7).

$$\Phi_{Em} = \Phi_0 \cdot Ex(\lambda_0) \cdot \alpha(\lambda_0) \quad (7)$$

*LightTools* then uses the emission spectrum for the absorbed wavelength ( $Em_{\lambda_0}(\lambda)$ ) and probabilistically chooses the outgoing wavelength and power from the *spectral power distribution* (SPD), which satisfies the condition shown in Equation (8), and a new ray is isotropically emitted from the particle.

$$\Phi_{Em} = \int_{-\infty}^{\infty} Em_{\lambda_0}(\lambda) d\lambda \quad (8)$$

It might appear as though Equation (7) and Equation (8) do not take into account any Stoke’s losses; but in fact, they do. Because the excitation spectrum is defined as the percentage of the absorbed power that becomes converted, the Stoke’s Shift and non-radiative losses become, as a percentage of the

absorbed power,  $1 - Ex(\lambda)$ . *LightTools* uses the excitation spectrum as a multiplicative factor; therefore, the ray’s power is reduced by the percentage that are the Stoke’s Shift and non-radiative losses.

### Power Balance using Quantum Yield

In this case, once the ray is absorbed by the phosphor particle, *LightTools* uses the quantum yield ( $QY(\lambda)$ ) to determine if the ray is re-emitted. As with the excitation spectrum, if  $QY(\lambda_0) = 0$  the ray stops at the particle and its power is lost. Otherwise, *LightTools* probabilistically chooses an outgoing wavelength ( $\lambda_1$ ) from the emission spectrum for the incoming wavelength. The power in the outgoing ray ( $\Phi_1$ ) is determined by the relation shown in Equation (9).

$$\Phi_1 = \Phi_0 \cdot \alpha(\lambda_0) \cdot QY(\lambda_0) \cdot \frac{\lambda_0}{\lambda_1} \quad (9)$$

where

$$\frac{\lambda_0}{\lambda_1} = \text{Stoke's Shift}$$

## Creating a Phosphor Material in the LightTools User Interface

The following three steps are used to create a phosphor material in *LightTools*.

1. Create a new User Material.
2. Add one or more Phosphor Particles to the new user material.
3. Specify the physical and optical properties of each of the phosphor particles.

Each of these steps will be elaborated upon in the subsequent sections.

### Step 1 - Adding a New User Material

With a model open in *LightTools*, choose **User Materials** from the **Edit** menu, as shown in Figure 5.

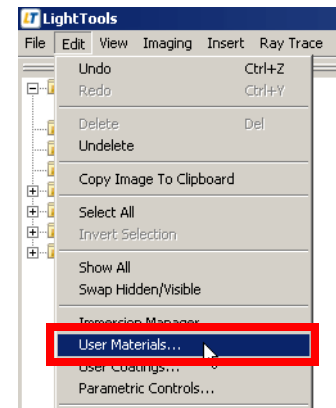


Figure 5. Choose Edit > User Materials to open the User Material dialog box.

In the resulting User Material dialog box, click the **Insert** button at the bottom-left corner as shown in Figure 6.

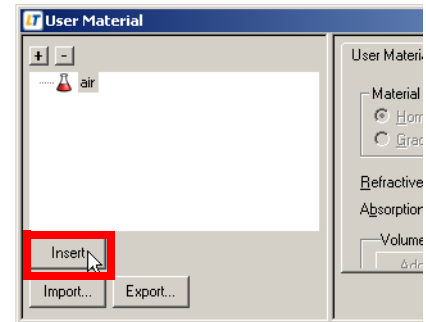
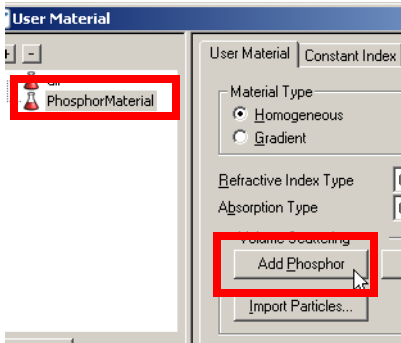


Figure 6. The Insert button adds a new user material to the list.

A new material is added to the list of user materials. You are prompted to change the name. The remainder of this tutorial uses a material arbitrarily named “PhosphorMaterial.”

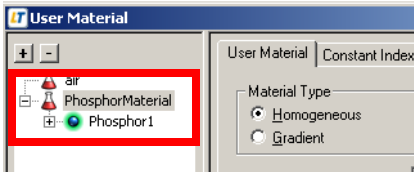
### Step 2 - Adding a Phosphor Particle to a User Material

To add phosphor particles to a user material, select the material in the User Material dialog box, then click the **Add Phosphor** button on the User Material tab, as shown in Figure 7.



**Figure 7. The Add Phosphor button adds a new phosphor particle to the user material.**

A phosphor particle is now a child of the user material in the tree as shown in Figure 8.



**Figure 8. The new phosphor particle appears as a child under the user material.**

You can add more than one type of phosphor particle to any user material by clicking the **Add Phosphor** button for each of the desired phosphors. Inert particles can be added to the material by clicking **Add Mie** or **Add User-Defined** buttons.

### Step 3 - Specifying the Phosphor Particle's Properties

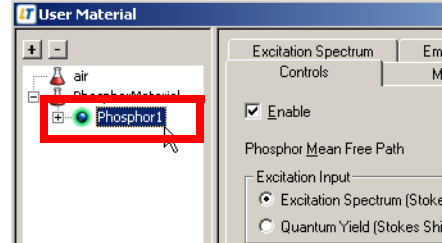
There are several required inputs for the *LightTools* phosphor particle. These inputs are as follows:

1. Mean Free Path
2. Absorption Spectrum
3. Excitation Spectrum/Quantum Yield
4. Emission Spectra
5. Intensity Distribution of Unconverted Energy
6. Number of Rays Propagating from a Particle

Each of these parameters must be specified in order to accurately model the phosphor. Many of the parameters are difficult to measure directly. "Measuring a Phosphor for use in *LightTools*" on

page 8 describes in detail how to measure a phosphor and convert the measured data into *LightTools* inputs.

To change any of the phosphor particle's options, select the phosphor child of the user material in the User Material dialog box as shown in Figure 9.



**Figure 9. Selecting the phosphor particle exposes its parameters.**

### Specifying the Phosphor Mean Free Path

The mean free path is the average distance (in millimeters) that a ray of light travels through the material without striking a phosphor particle. It can be calculated using the effective cross-sectional area ( $\text{mm}^2$ ) of a phosphor particle and the number of phosphor particles per unit volume ( $1/\text{mm}^3$ ) of the host material, also known as the density of particles, as shown in Equation (10).

$$\ell = \frac{1}{n\sigma_{eff}} \quad (10)$$

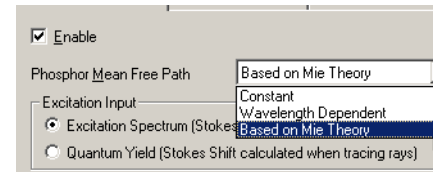
where

$\ell$  = mean free path

$n$  = density of particles

$\sigma_{eff}$  = effective cross-sectional area

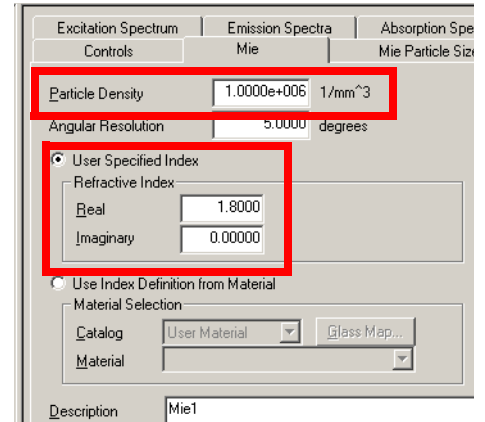
There are three options for inputting the mean free path into *LightTools*, as shown in Figure 10.



**Figure 10. The mean free path can be specified as a constant value, with wavelength dependence, or based upon Mie theory.**

The default option, Based on Mie Theory, uses a well-known volumetric scattering theory to calculate the mean free

path based upon the density of a distribution of spherical particles of given sizes with a given index of refraction. To use Based on Mie Theory, enter the particle density and refractive index on the Mie tab as shown in Figure 11.



**Figure 11. The particle's density and index of refraction must be specified on the Mie tab.**

You can enter a complex index of refraction for the Mie particles; using an imaginary component implies that the particle absorbs light, which would conflict with the absorption spectrum already supplied for the phosphor. For the purpose of a phosphor that uses any Mie parameters, the absorption due to the particles complex refractive index is ignored.

When using the Mie solution to calculate mean free path by particles with a complex refractive index, Equation (10) changes to compensate for the absorption cross-sectional area. The resulting equation, Equation (11), also shows the wavelength dependence of the scattering cross-sectional area and the absorption cross-sectional area.

$$\ell = \frac{1}{n(\sigma_{scat} + \sigma_{abs})} \quad (11)$$

where

$\ell$  = mean free path

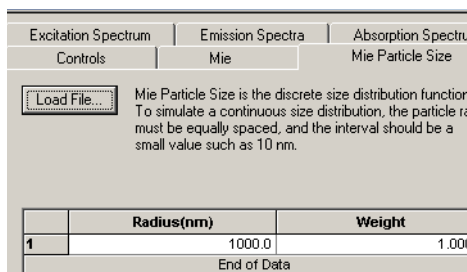
$n$  = density of particles

$\sigma_{scat}$  = scattering cross-sectional area

$\sigma_{abs}$  = absorption cross-sectional area

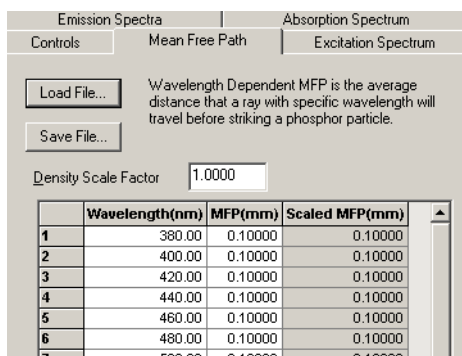
Also, the size distribution of the particles must be specified on the Mie Particle Size tab as shown in Figure 12. The

Mie solution assumes that the particles are small spheres, so the size of the particles is represented by their radii. The particle size distribution can be loaded from an external file. The format for the file is shown in Figure 24 on page 7.



**Figure 12. The particle size distribution is entered on the Mie Particle Size tab.**

When the Constant mean free path is chosen, a single value is entered on the Mean Free Path tab. If Wavelength Dependent is chosen, the Mean Free Path tab contains a table of values and their corresponding wavelengths, as shown in Figure 13.



**Figure 13. The mean free path can have wavelength dependence.**

The data can be entered manually, or an external text file can be used. The format for the text file is given in Figure 25 on page 7.

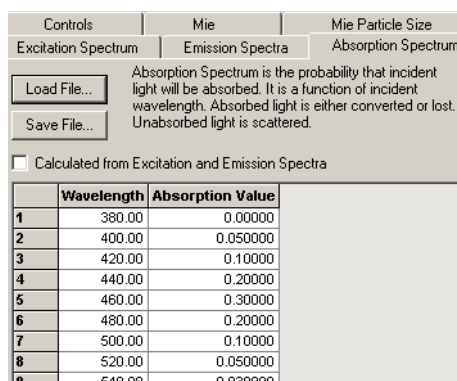
A Density Scale Factor can be entered on this tab to change the absolute values of all of the mean free paths without shifting the relative shape of the curve. The scale factor is applied as if the particle density is being changed. From Equation (10), the mean free path and the particle density have an inverse relationship; assuming a constant particle size, if the density is doubled, the mean free path is halved. This allows you to change or optimize on the density,

which is easier to measure, while using a wavelength-dependent mean free path.

### Absorption Spectrum

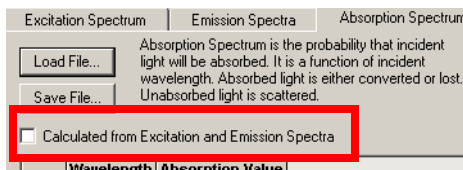
The absorption spectrum,  $\alpha(\lambda)$ , is the wavelength-dependent probability function that light striking a phosphor particle will be absorbed. The wavelengths used to define the absorption spectrum should be a subset of the wavelengths traced in the *LightTools* model. Spectrum values range from 0 to 1, where a value of 1 indicates that 100% of the rays with the corresponding wavelength are absorbed by a phosphor particle.

You can enter the wavelength-dependent absorption spectrum into the table on the Absorption Spectrum tab manually, as shown in Figure 14, or a text file can be defined to enter all of the values at once. The format needed for the text file is shown in Figure 28 on page 8.



**Figure 14. The Absorption Spectrum tab**

You can also allow *LightTools* to calculate the absorption spectrum based upon the emission spectra and the excitation spectrum/quantum yield. If you choose the “Calculated from Excitation and Emission Spectra” option on the Absorption Spectrum tab, as shown in Figure 15, you do not need to specify the absorption spectrum.



**Figure 15. The Calculated from Excitation and Emission Spectra option calculates the absorption spectrum automatically.**

In this case, the excitation spectrum/quantum yield and emission spectra are used to determine the absorption spectrum, as shown in Equation (12). When using quantum yield, substitute *QY* for *Ex* in Equation (12).

$$\alpha(\lambda) = \frac{Ex(\lambda)}{Ex(\lambda) + Em(\lambda)} \quad (12)$$

This specification ensures that any ray whose wavelength corresponds to a non-zero value in the excitation spectrum is absorbed and also re-emitted. It is important to note that Equation (12) is dependent on the emission spectrum only if there is overlap between the emission spectrum and its excitation wavelength.

### Excitation Spectrum/Quantum Yield

The excitation spectrum and the quantum yield are the wavelength-dependent relations that define what percentage of absorbed light of a particular wavelength is re-emitted. The set of wavelengths that define the excitation spectrum or the quantum yield should be within the range of wavelengths in the absorption spectrum. The excitation spectrum values can be any positive number from 0 to  $\infty$ , with a value of 1 indicating that 100% of the absorbed light is converted by the phosphor.

Quantum yield is also defined from 0 to  $\infty$ ; however, unlike the excitation spectrum, a value of 1 indicates that the only losses in the system are due to Stoke’s Shift.

The data for both of these types exists in *LightTools* in tabular format, with one row per wavelength that contains the wavelength value and the conversion percentage at that wavelength. A user can enter each of the rows manually, or load a text file that allows all of the data to be entered at once. The format for the input excitation spectrum data file is shown in Figure 26 on page 7. The format for the input quantum yield data file is shown in Figure 27 on page 7.

Figure 16 shows the Excitation Spectrum tab. Figure 17 shows the Quantum Yield tab.

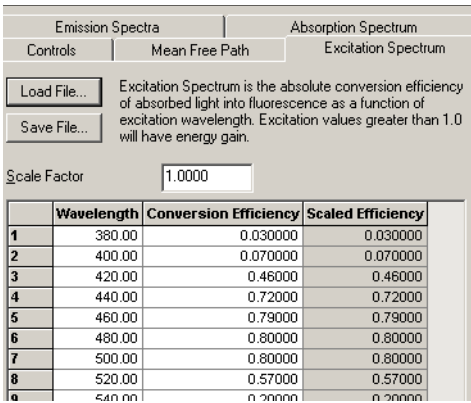


Figure 16. The Excitation Spectrum tab

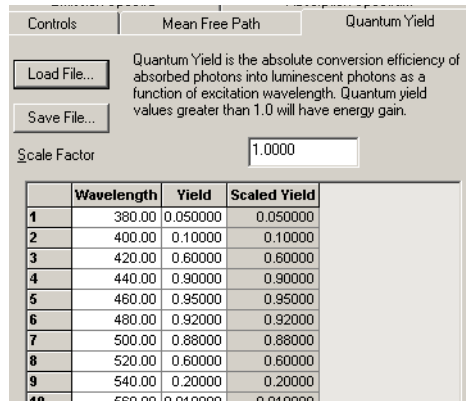


Figure 17. The Quantum Yield tab

Both the Excitation Spectrum and the Quantum Yield tabs have a field labeled Scale Factor. In both of these cases, the Scale Factor directly modifies the absolute values of the data in the table without modifying the relative shape. The scale factor is useful if you are using data that has been normalized and you need to convert it to absolute values. In this case, enter the normalized values into the *LightTools* table, then set the scale factor equal to the desired peak value.

### Emission Spectra

The emission spectra, which define the spectrum of light emitted for any absorbed wavelength, must also be specified. The tab that contains the emission spectra data is shown in Figure 18. This data can be entered manually or via a text file, the format for which is shown in Figure 29 on page 8.

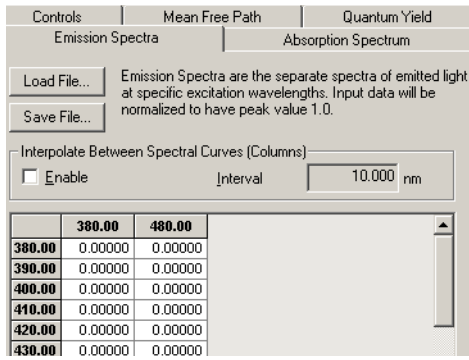


Figure 18. The Emission Spectra tab

The data on the Emission Spectra tab is organized into columns that represent the emission spectrum vs. emission wavelength at a particular absorbed wavelength. You can insert a new emission spectrum by selecting a column header, right-clicking, and choosing Insert Column, as shown in Figure 19.

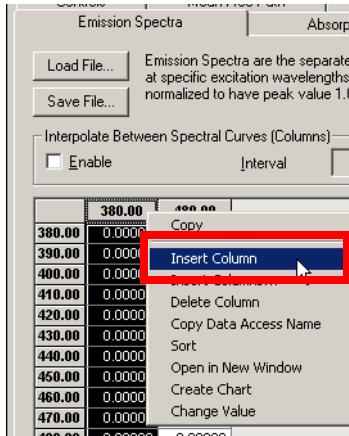


Figure 19. Inserting a new emission spectrum

By default, if an absorbed ray is of a wavelength that does not have a corresponding column on this tab, *LightTools* will use the emission spectrum whose absorbed wavelength is closest to the current ray's. If the Interpolate Between Spectral Curves (Columns) option is enabled, *LightTools* generates new, interpolated spectra at every Interval and uses the closest interpolated spectrum for the current ray.

### Unconverted Intensity

When a ray is absorbed and re-emitted from the phosphor, it does so isotropically. If the ray is not absorbed when it strikes the phosphor particle, it propagates away from the particle as defined

by the Intensity Distribution for Unconverted Rays control on the Controls tab for the phosphor particle.

There are four options for this setting, as shown in Figure 20. The default option, Isotropic, scatters the energy equally in all directions. With the Undeviated option, the ray passes through the particle as if there was no interaction at all. This option can be used to model luminescent dyes, such as for laser or solar applications.

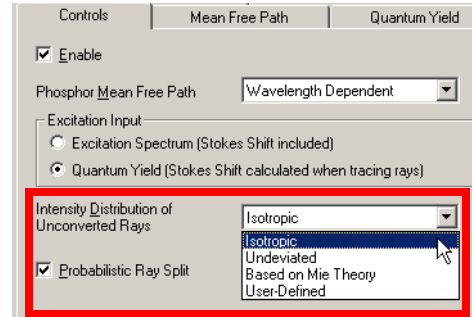


Figure 20. Options for the Intensity Distribution of Unconverted Rays

If you select the Based on Mie Theory, the intensity distribution is calculated using the Mie solution. If you are already using Mie inputs for the mean free path, the same inputs will be used for the unconverted intensity calculation.

The last type, User Defined, allows you to manually specify the intensity distribution. This option could be used to enter a measured distribution. The intensity as a function of wavelength and angle is entered on the Unconverted Intensity tab, shown in Figure 21.

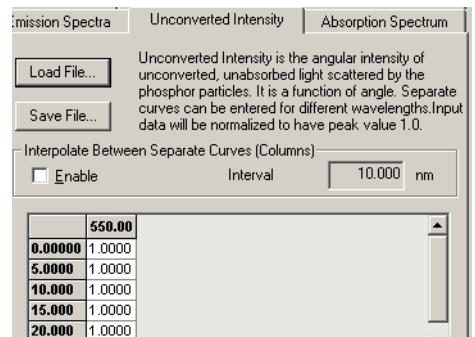
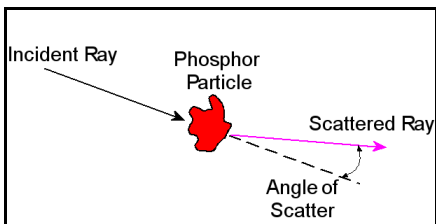


Figure 21. Specifying a user defined intensity distribution

The table consists of one column per wavelength and one row per angle. The

angle is specified with respect to the undeviated direction, as shown in Figure 22.

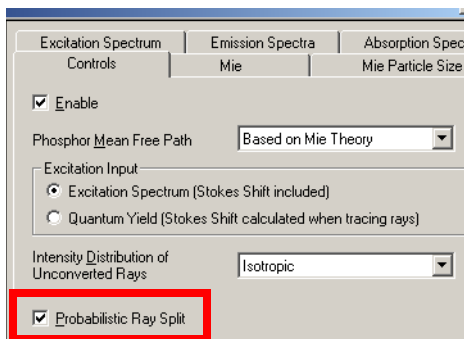


**Figure 22. Graphical depiction of the unconverted intensity scatter angle**

The Interpolate Between Separate Curves (Columns) option works the same way as the similar control on the Emission Spectra tab. See “Emission Spectra” on page 6 for more information. The data in this table can also be loaded from an external file. The format for the file is shown in Figure 30 on page 8.

### Number of Rays Propagating from the Particle

The last control that must be considered for the phosphor particle is labeled Probabilistic Ray Split on the Controls tab of the particle definition, as shown in Figure 23. By default, *LightTools* propagates one ray away from the particle. If there is no conversion, this ray is the unconverted ray. If there is conversion, *LightTools* probabilistically chooses whether to propagate the converted or unconverted ray. If this option is unchecked, when conversion occurs, two rays propagate from the particle: the converted and the unconverted ray. Using this option speeds up the ray trace, as fewer rays propagate through the system.



**Figure 23. The Probabilistic Ray Split option controls how many rays propagate from the phosphor particle.**

## File Formats for Phosphor Data

Many of the required inputs for the phosphor particles are tables of data. You can always enter the data manually or copy it from the clipboard, but it is often convenient to load this data from external files. As such, all of the phosphor data tables in *LightTools* have a Load File button. This section describes the file formats associated with each of the tabular data sets.

### Mie Particle Size

The Mie particle size data can be loaded from a file organized as shown in Figure 24. The weight values do not need to be normalized, as this is done by *LightTools* during the simulation.

```
dfat version 1.0
dataname: Mie Particle Size Data
DATAPAIRS: radius weight
1000.0 1.0
1100.0 2.0
1200.0 3.0
1300.0 4.0
... ..
```

**Figure 24. Mie Particle Size file format**

The radius values in the file are always in nanometer units, regardless of the system units of the *LightTools* model.

### Wavelength Dependent Mean Free Path

The file format for the mean free path as a function of wavelength is shown in Figure 25. The mean free path values are always specified in millimeters (mm), regardless of system units.

```
dfat version 1.0
dataname: Wavelength-dependent MFP
DATAPAIRS: wv MFP
380 0.1
400 0.1
420 0.1
440 0.1
... ..
```

**Figure 25. Wavelength Dependent Mean Free Path file format**

## Excitation Spectrum

The excitation spectrum can be loaded from a file with the format shown in Figure 26.

```
dfat version 1.0
dataname: Excitation Spectrum
DATAPAIRS: wv inten
380 0.03
400 0.07
420 0.46
440 0.72
... ..
```

**Figure 26. Excitation Spectrum file format**

The intensity values in the file are absolute conversion values; a value greater than one implies that more energy leaves the particle than was incident upon it.

### Quantum Yield

The quantum yield values can be brought into *LightTools* via a file with the format shown in Figure 27.

```
dfat version 1.0
dataname: Quantum Yield
DATAPAIRS: wv yield
380 0.05
400 0.10
420 0.60
440 0.90
... ..
```

**Figure 27. Quantum Yield file format**

The yield values in the file are absolute quantum yield values. A value of 0 means that there is no conversion at that wavelength; a value of 1 implies that the only losses at that wavelength are due to Stoke’s Shift.

### Absorption Spectrum

The absorption spectrum’s file format is shown in Figure 28. The intensity values in this file are probabilities. As such all values should be between 0 and 1.

*LightTools* interpolates between the data points in the table for undefined wavelengths. It is important to define wavelengths that have a zero absorption factor to ensure that the interpolation

routine calculates the absorption factor to be zero beyond the domain of the defined data.

```
dfat version 1.0
dataname: Absorption Spectrum
DATAPAIRS: wv inten
380    0.00
400    0.05
420    0.10
440    0.20
...    ...
```

**Figure 28. Absorption Spectrum file format**

### Emission Spectra

The emission spectra can be loaded all at once from a file of the format shown in Figure 29.

```
dfat version 1.0
dataname: Emission Spectra
DATAPAIRS: wv inten
DATASETS: 2
        380    480
480    0.000  0.000
490    0.275  0.275
500    0.498  0.498
510    0.705  0.705
...    ...    ...
```

**Figure 29. Emission Spectra file format**

Each column of the tab-delimited data set is the emission spectrum associated with a particular absorbed wavelength. The DATASETS parameter identifies the number of absorbed wavelengths and, consequently, how many columns of data, the file contains. The row immediately below the DATASETS parameter identifies the absorbed wavelengths. The left-most value in this list corresponds to the left-most emission spectrum.

In order to ensure proper interpolation between the columns and the data points within a column, it is important to make sure that the data in each column start and end with zero values.

### User Defined Unconverted Intensity Distribution

User defined unconverted intensity files must be of the form shown in Figure 30.

```
dfat version 1.0
dataname: Unconverted Intensity
DATAPAIRS: angle inten
DATASETS: 1
        550
0      1
5      1
10     1
15     1
...    ...
```

**Figure 30. User Defined Unconverted Intensity file format**

As with the emission spectra, this file can contain multiple columns of data: one for each of the defined wavelengths. The DATASETS parameter identifies how many columns of data are present in the file. The line immediately following the DATASETS line lists the wavelengths associated with each of the columns.

### Measuring a Phosphor for use in LightTools

As you can see from the preceding sections, many inputs are required to build a proper phosphor model. In summary, the necessary inputs are:

1. the absorption spectrum,
2. the excitation spectrum/quantum yield,
3. the mean free path,
4. the emission spectra, and
5. the refractive index of the phosphor.

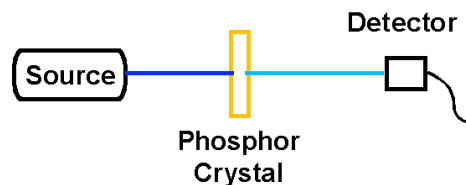
Luckily, the first three inputs can be calculated from a simple *inline transmission* measurement. This section discusses how to obtain the necessary phosphor inputs. See “Creating an LED Phosphor Model from Measured Data” on page 10 to learn how these parameters are applied to various phosphor applications.

### Obtaining Inline Transmission

The inline transmission ( $T_i(\lambda)$ ) is a convenient measurement that can be used to derive many of the required inputs for a phosphor model. From this wavelength dependent set of values, the absorption spectrum, the mean free path, and the excitation spectrum/quantum yield can be computed. There are several ways to obtain the data.

#### Measuring Inline Transmission

To measure the inline transmission, a wavelength-tunable, well-collimated source is required. Light from this source is directed onto a single phosphor crystal at normal incidence. A detector on the opposite side of the crystal from the source collects the power transmitted through the material as shown in Figure 31.



**Figure 31. Graphical depiction of an inline transmission measurement system**

By scanning the source through a series of wavelengths, a set of input and transmitted power can be obtained. The inline transmission is simply the ratio of the transmitted power to the input power.

#### Deriving Inline Transmission from a Complex Refractive Index

The complex refractive index of the phosphor crystal, as shown in Equation (13), can be used to calculate inline transmission using the extinction coefficient and Equation (14).

$$\hat{n}(\lambda) = n(\lambda) + ik(\lambda) \quad (13)$$

where

$n(\lambda)$  = index of refraction

$k(\lambda)$  = extinction coefficient

$$T_i(\lambda) = e^{-\frac{4\pi k(\lambda)D}{\lambda}} \quad (14)$$

where

$D$  = Sample Thickness

$k(\lambda)$  = Extinction Coefficient

### Deriving Inline Transmission from Absorbance

In some cases, the absorbance of the phosphor crystal is given. You can use Equation (15) to convert the absorbance to the inline transmission.

$$T_i(\lambda) = 10^{-\text{absorbance}(\lambda)} \quad (15)$$

### Calculating the Bulk Transmission of the Phosphor Crystal

To calculate a phosphor materials' properties, the internal or bulk transmission of the crystal is needed. The inline transmission contains the bulk transmission ( $T_b$ ) as well as the losses due to Fresnel reflectance at each of the faces of the crystal. Equation (16) shows the relationship between the bulk transmission, the inline transmission, and the total Fresnel transmission ( $T_F$ ).

$$T_i(\lambda) = T_b(\lambda) \cdot T_F(\lambda) \quad (16)$$

The total Fresnel transmission is related to the total Fresnel reflectance ( $R_F$ ) by Equation (17).

$$T_F(\lambda) = 1 - R_F(\lambda) \quad (17)$$

The total Fresnel reflectance is the reflectance due to the 1st and 2nd surface intersections as well as the infinite other back reflections. The total Fresnel reflectance relates to the Fresnel reflectance of one surface ( $R_{1F}$ ) by Equation (18).

$$R_F(\lambda) = \frac{2R_{1F}(\lambda)}{1 + R_{1F}(\lambda)} \quad (18)$$

For normal incidence, the Fresnel reflectance due to a single surface interaction is given by Equation (19) using only the wavelength-dependent refractive index.

$$R_{1F}(\lambda) = \left( \frac{1 - n(\lambda)}{1 + n(\lambda)} \right)^2 \quad (19)$$

The contribution to the total Fresnel transmission of the high order reflections is small. Consequently, a good approximation for Equation (17) is given in Equation (20).

$$T_F(\lambda) = T_{1F}(\lambda)^2 \quad (20)$$

where

$$T_{1F}(\lambda) = 1 - R_{1F}(\lambda)$$

### Calculating the Absorption Spectrum and the Mean Free Path

Armed with the bulk transmission from the previous section, you can now calculate the absorption spectrum and the mean free path of the phosphor crystal. Equation (21) shows the relationship between all of these values. In Equation (21), the absorption is shown to be wavelength dependent. You can also choose to have a single absorption value and let the mean free path vary with wavelength.

$$T_b(\lambda) = e^{-\frac{D \cdot \alpha(\lambda)}{\ell}} \quad (21)$$

where

$D$  = Sample Thickness

$\alpha(\lambda)$  = Absorption Spectrum

$\ell$  = Mean Free Path

It follows then that the absorption spectrum definition is given by Equation (22).

$$\alpha(\lambda) = -\frac{\ell \cdot \ln(T_b(\lambda))}{D} \quad (22)$$

Since the absorption spectrum is a probability distribution, and we want the best probability that the phosphor will work as expected, the absorption spectrum must be normalized. From Equation (22), it can be shown that the maximum of the absorption spectrum occurs at the minimum value of the bulk transmission. Using this concept gives Equation (23).

$$\alpha_{max} = -\frac{\ell \cdot \ln(T_{b-min})}{D} \quad (23)$$

Setting the maximum absorption spectrum value equal to 1 allows us to solve for the mean free path, as shown in Equation (24).

$$\ell = -\frac{D}{\ln(T_{b-min})} \quad (24)$$

### Obtaining the Quantum Yield

The best quantum yield value to use when modeling phosphors is one given by the manufacturer. The quantum yield need only be a single value because as we've defined it, the absorption spectrum contains all of the spectral information. Often, a quantum yield of 0.92 is reasonable if no other value can be obtained or determined.

### Calculating the Quantum Yield from the Inline Transmission

If the quantum yield value is not given, you can derive it from the inline transmission. To understand how to calculate the quantum yield value, consider the inline transmission measurement system's energy balance. The incident power ( $\Phi_0$ ) is comprised of the absorbed power ( $\Phi_\alpha$ ), the power lost to Fresnel reflections ( $\Phi_F$ ), and the unabsorbed power ( $\Phi_{un\alpha}$ ) as shown in Equation (25).

$$\Phi_0 = \Phi_\alpha + \Phi_F + \Phi_{un\alpha} \quad (25)$$

The re-emitted power ( $\Phi_{Em}$ ), given by the absorbed power scaled by the quantum yield value and the Stoke's Shift, is the integrated spectral power distribution as shown in Equation (26).

$$\Phi_{Em} = QY \cdot \Phi_\alpha \cdot SS \quad (26)$$

where

$SS$  = Stoke's Shift

$$\Phi_{Em} = \int_{-\infty}^{\infty} Em_{\lambda_0}(\lambda) d\lambda$$

The total emitted power cannot be obtained directly from the inline transmission measurement. Instead, an inte-

grating sphere and a spectrometer must be used to capture and measure the isotropically-emitted radiation.

To calculate the Stoke's Shift, a weighted average of the emitted wavelengths should be used. Equation (27) shows the nominal relationship for the Stoke's Shift and the weighting used to calculate the emitted wavelength from the emission spectrum.

$$SS = \frac{\lambda_0}{\lambda_1} \quad (27)$$

where

$$\lambda_1 = \frac{1}{N} \sum_{i=1}^N \lambda_i \cdot Em_{\lambda_0}(\lambda_i)$$

If you are using un-normalized values for the emission spectrum, Equation (27) becomes:

$$SS = \frac{\lambda_0 \Phi_{Em}}{N \sum_{i=1}^N \lambda_i \cdot Em_{\lambda_0}(\lambda_i)} \quad (28)$$

Combining Equation (25) and Equation (26) while dividing by  $\Phi_0$  gives Equation (29).

$$1 = \frac{\Phi_{Em}}{\Phi_0 \cdot QY \cdot SS} + \frac{\Phi_F}{\Phi_0} + \frac{\Phi_{un\alpha}}{\Phi_0} \quad (29)$$

You might notice that the last addend in Equation (29) is the inline transmission ( $T_i$ ). The second to last term is the total Fresnel reflectivity ( $R_F$ ). Substituting these values into Equation (29) gives Equation (30), the equation for the quantum yield value.

$$QY = \frac{\Phi_{Em}}{\Phi_0 \cdot SS} (1 - R_F - T_i)^{-1} \quad (30)$$

It is important to note that in order to properly derive the quantum yield, the absorbed wavelength ( $\lambda_0$ ) and the emission spectrum for that wavelength should not overlap. The calculation of the converted power ( $\Phi_{Em}$ ) would be skewed.

## Obtaining the Emission Spectra

Of all of the parameters that define a phosphor material, the emission spectra is the most likely to be given on a data sheet. You can also measure the emission spectrum with an integrating sphere and a spectrometer.

## Creating an LED Phosphor Model from Measured Data

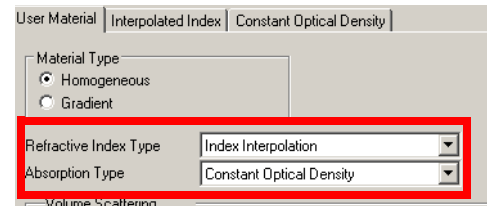
There are two primary ways in which to use a phosphor inside of an LED: using a single, cut phosphor crystal or using a particular density of small phosphor particles suspended in an encapsulant.

When using a single crystal, the measured data obtained in the previous section can be used directly as inputs, but when the phosphor particles are in suspension, extra steps must be taken to ensure that a good model is achieved. This section describes the process for creating each of these two phosphor models.

## For a Single Phosphor Crystal

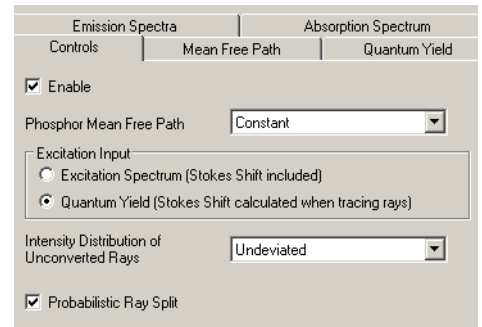
The inline transmission of the previous section is of a single crystal, and as such, the data derived from it can be used directly as *LightTools* inputs. To create this kind of phosphor material, first follow Steps 1 and 2 as described in "Creating a Phosphor Material in the *LightTools* User Interface" on page 3 to add a new material with phosphor particles to the *LightTools* model.

Change the Refractive Index Type of the base material to whatever formulation you have for the phosphor crystal. In many cases, this may just be Index Interpolation. Set the Absorption Type to Constant Optical Density. The default optical density of zero is correct, since we want the phosphor particles absorption to dictate all of the losses in the material. These settings are show in Figure 32.



**Figure 32. Refractive Index and Absorption Type for a Single Phosphor Crystal**

Next, on the properties page for the phosphor particle, as shown in Figure 33, set the Phosphor Mean Free Path to be Constant. Choose Quantum Yield or Excitation Spectrum, depending on which of these values you have. Also choose Undeviated for the Intensity Distribution of Unconverted Rays.



**Figure 33. Phosphor particle settings for a single phosphor crystal**

For the absorption spectrum, as shown in Figure 14 on page 5, use the data that you calculated using Equation (22). The constant mean free path is the value given by Equation (24). The quantum yield or excitation spectrum value is the given value. Lastly, the measured emission spectrum should be entered into the Emission Spectra tab, as shown in Figure 18 on page 6.

It is important to note that Equation (21) can be solved with a wavelength-dependent absorption or mean free path. This example assumes that the absorption varies with mean free path, but using the wavelength-dependent mean free path is equally valid. In this case, you simply choose the Wavelength Dependent mean free path instead of Constant, and enter the data.

## For Phosphor Particles in Suspension

When the phosphor particles are suspended in an encapsulant, the model becomes more difficult. In addition to the need to accurately model all aspects of the phosphor, the properties of the encapsulant must also be taken into account. To accurately model this case, three separate material models will be created; the first two act as references used to create the third.

### Creating the Single Crystal Material

The first reference material to create is the single phosphor crystal material. This material will use the refractive index and absorption properties as measured or derived for the single phosphor crystal without using a phosphor particle. To create this reference material, first add a new material as described in “Step 1 - Adding a New User Material” on page 3. Name this new material “SingleCrystal.” Change the Refractive Index Type to match the available data and the Absorption Type to Transmittance vs. Length as shown in Figure 34.

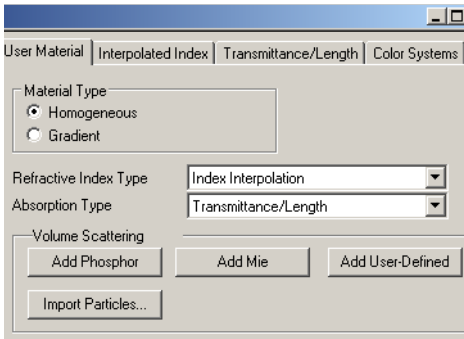


Figure 34. Single crystal reference material settings

The refractive index should be entered according to the type of data you have. The transmittance vs. length data is the internal transmission of the bulk material. Use the  $T_b$  as calculated by Equation (16). The “At Length” parameter in *LightTools* (Figure 35), is the thickness of the sample used for the inline transmission measurement.

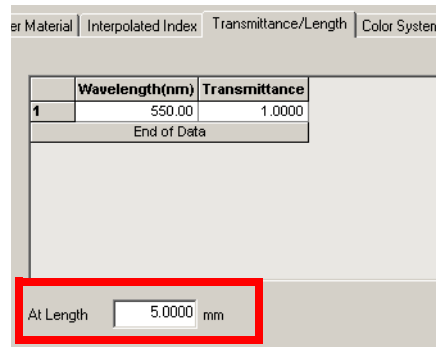


Figure 35. Transmittance vs. Length parameters

### Creating the Mie Scattering Material

The second reference material will be used to calculate the phosphor particle absorption spectrum for the phosphor particles using a simple Mie scatterer. When the phosphor particles are in suspension, there are several types of absorption present: the encapsulant material, the absorption within the phosphor particle, and the losses due to interactions with the absorbing phosphor particles. The material model in *LightTools* needs to account for all of these.

Create a new user material and name it “MieReference,” using the process described in “Step 1 - Adding a New User Material” on page 3. Enter the refractive index and absorption information for the base material. This information is NOT the same as the phosphor material. For LEDs, this material is commonly a silicone. For reference, one such type of LED encapsulant is LS-3140 from NuSil Technology at:

<http://www.nusil.com>

Add a new Mie particle by selecting the “Add Mie” button on the User Material tab as seen in Figure 36.

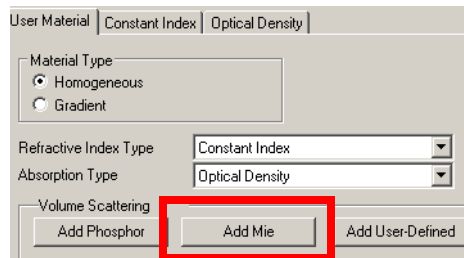


Figure 36. The Add Mie button

A new Mie particle set is added to the material. On the Controls tab for the Mie particles, enter the Particle Density of the phosphor particles and change the refractive index type to Use Index Definition from Material. Select the reference material created in the last section from the list of available user materials as shown in Figure 37.

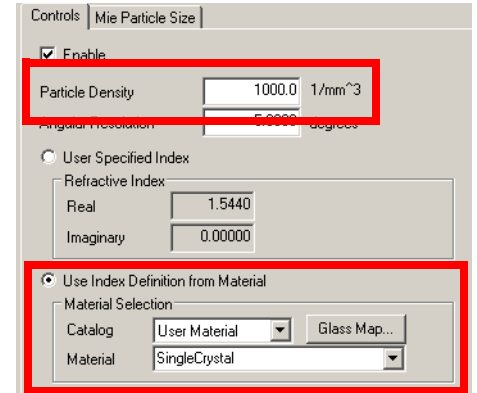


Figure 37. Enter the Mie particle density and use the first reference material for the particle’s refractive index.

Finally, define the particle size distribution on the Mie Particle Size tab. It is usually best to use a set of sizes, instead of a single particle size. Since most size distributions follow a normal, or gaussian, curve, you can use Equation (31) with a small standard deviation as the set of particle sizes.

$$size(x) = e^{-\frac{(x-\mu)^2}{2\sigma^2}} \quad (31)$$

where

$\mu$  = Average Size

$\sigma$  = Standard Deviation

Once all of the Mie data is entered, switch to the Mie evaluator child of the Mie particle as shown in Figure 38.

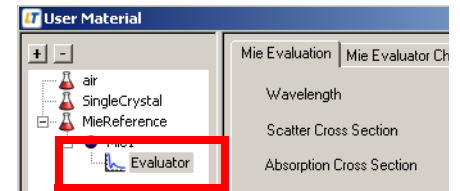
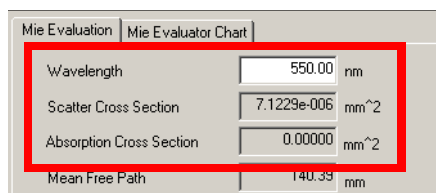


Figure 38. The Mie evaluator

On the Mie Evaluation tab, the three important fields are the editable field “Wavelength” and the two un-editable

fields labeled “Scatter Cross Section” and “Absorption Cross Section.” as shown in Figure 39.



**Figure 39. The important Mie evaluator tab fields**

These three fields will be used to build the absorption spectrum for the phosphor particles based upon Equation (32).

$$\alpha(\lambda) = \frac{\sigma_{\alpha}(\lambda)}{\sigma_{\alpha}(\lambda) + \sigma_{scatter}(\lambda)} \quad (32)$$

where

$\sigma_{\alpha}(\lambda)$  = Absorption Cross Section

$\sigma_{scat}(\lambda)$  = Scatter Cross Section

Because the absorption spectrum should have a large number of wavelengths, the best way to scan through the wavelengths is by writing and using a Macro.

### **Creating the Phosphor Material for use in the LED**

With a new absorption spectrum calculated, you can now create the phosphor material that will be used in your LED model. First, create a new user material and assign the optical properties of the encapsulant material as you did in “Creating the Mie Scattering Material” on

page 11, but do not add the Mie scattering particles. Instead, add a phosphor particle as described in “Step 2 - Adding a Phosphor Particle to a User Material” on page 3.

Set the Mean Free Path of the phosphor particles to be Based on Mie Theory as shown in Figure 10 on page 4. Set the Mie Particle Density to the desired value, and change the Refractive Index of the Mie phosphor particles to use the Index Definition of the first reference material you created. Figure 37 on page 11 depicts these settings. Also enter the same particle size distribution on the Mie Particle Size tab that you used for the second reference material. It is important to note that the absorption of the first reference material is not considered part of the phosphor material’s energy balance, as it conflicts with the phosphor particles’s absorption spectrum.

Next, enter the optical properties of the phosphor particles. The absorption spectrum is the data you calculated from Equation (32). The emission spectrum is the measured data. The quantum yield or excitation spectrum is the value as discussed in “Obtaining the Quantum Yield” on page 9.

Finally, change the Intensity Distribution of Unconverted Rays to be Based on Mie Theory, as shown in Figure 20 on page 6. Since all of the Mie parameters were previously entered, nothing

else needs to be done. The material is ready to use.

## **Conclusion**

The interaction of light with a phosphor material is a complicated physical and optical process. This complexity manifests itself in the software model as well. *LightTools* has many inputs to its model in order to allow you to create a wide variety of fluorescent materials, the most common of which in illumination systems is a phosphor for use in white-LEDs. This white paper describes the *LightTools* inputs for the phosphor materials in “Creating a Phosphor Material in the LightTools User Interface” on page 3.

In addition to the complex model inputs, the availability of the requisite data is such that you might have to measure the data for yourself. “Measuring a Phosphor for use in LightTools” on page 8 describes a measurement and a series of conversions to obtain the *LightTools* inputs. However, especially for LED phosphor systems, the method in which the phosphor model is built depends greatly on the physical application of the phosphor. “Creating an LED Phosphor Model from Measured Data” on page 10 discusses two possible scenarios for an LED phosphor and how to create the best *LightTools* model for each.

# O P T I C A L R E S E A R C H A S S O C I A T E S

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