

Introduction

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 2 shows, in simplified terms, the process of photoluminescence.

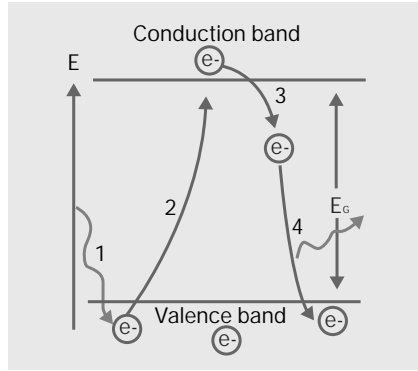


Figure 2: The process of photoluminescence

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).

Equation 1

$$E = \frac{hc}{\lambda}$$

where
 $h = \text{Planck's Constant}$
 $c = \text{speed of light}$
 $\lambda = \text{wavelength}$

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 equal to the exact 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.

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

Equation 5



The simulations performed in LightTools accurately depict the state of energy for a single moment in time. Because energy can vary per unit time. With this distinction in mind, Equation (5) becomes:

Equation 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 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

A ray 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

LightTools then uses the emission spectrum for the absorbed wavelength (E_{λ}), the emission 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.

Equation 8

$$E_{\lambda} = \Psi_{Em} \cdot \int_{-\infty}^{\infty} E_{\lambda_0}(\lambda) d\lambda$$

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,

and non-radiative losses.

Power Balance using Quantum Yield

The quantum yield is defined as the ratio of the number of photons emitted to the number of photons absorbed.

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

Step 3: Specifying the Phosphor Particle's Properties

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

4. Mean Free Path
5. Absorption Spectrum
6. Excitation Spectrum/Quantum Yield
7. Emission Spectra
8. λ gXaf'g' 7'f'g'Uhgba'bYHaVbai XegXW8aXeZl
9. 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 convert the measured data into LightTools inputs.

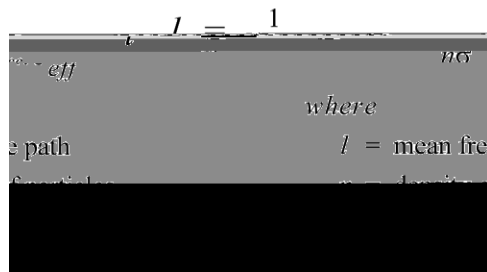
GbV[TaZXTal 'bYg' X'c[bfc[becTegV_Xf 'bcg'ba'f'Z'f'X_XVgg' X'c[bfc[beV[\WbYg' X'hfXe' TgXeT_'a'g' X'HfXe@TgXeT_WT_bZ 'Ubk Tf' shown in Figure 9.



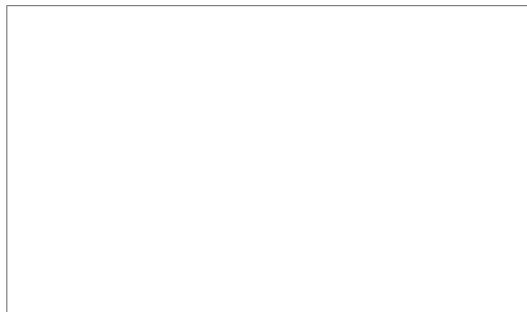
Figure 9: Selecting the phosphor particle exposes its parameters

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 (mm^2) of a phosphor particle and the number of phosphor particles per unit volume ($1/\text{mm}^3$)

Equation 10



G[XeXTeX'g eXX'bcgbaf 'Ybe'achggaZ 'g X'' XTa 'YeXX'cTg 'agp'?Z[gGbb_fZTf f[bj a'a'9ZheX'\$#!



$$l = \frac{1}{n(\sigma_{scat} + \sigma_{abs})}$$

where

l = mean free path
 n = density of particles
 σ_{scat} = scattering cross-sectional area
 σ_{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 on page 14? Please check this.

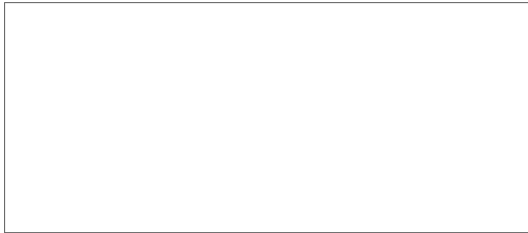


Figure 12: The particle size distribution is entered on the Mie Particle Size tab

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.

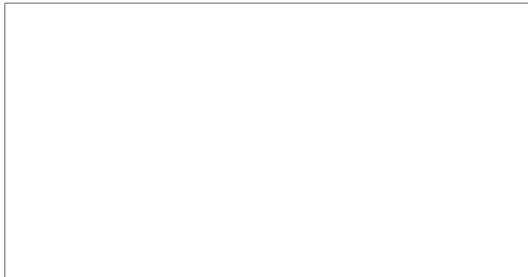


Figure 13: The mean free path can have wavelength dependence

The data can be entered manually, or an external text file can be used. The format for the text file is given on page 14.

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 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.

The wavelengths used to define the absorption spectrum should be a subset of the wavelengths traced in the LightTools 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 on page 15.

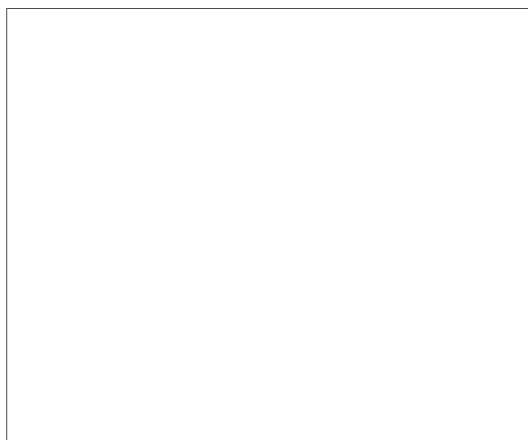


Figure 14: The Absorption Spectrum tab

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.



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.

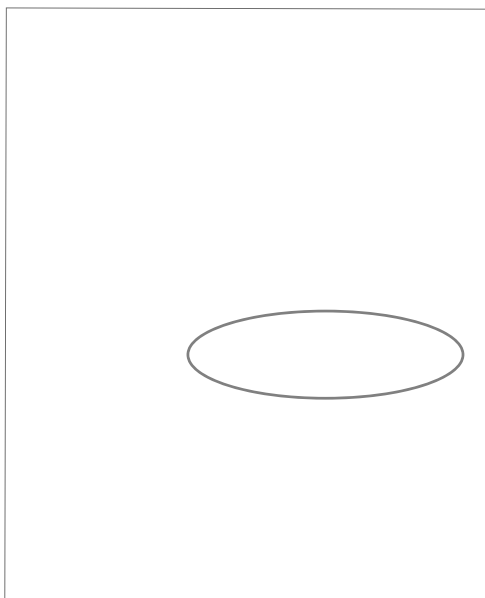


Figure 19: Inserting a new emission spectrum

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.

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, it passes through the phosphor. For more information on the phosphor particle, see the Controls tab for the phosphor particle.

luminescent dyes, such as for laser or solar applications.



G[X`_I fgg cXZhfXe7XYaXWZT_bj f`l bh'p` TahT_ f`cXVM` g`X`agXaf`g` WfgeUhgba!G[f`bcgba Vbh_WUX'hfXWp` XagXeT` XTfhXW WfgeUhgba!G[X`agXaf`g` Tf T`YhaVgba`bYj Ti X_XaZg` TaWTaZ_X`f` XagXeWba`g` X`HaVbai XegKW-agXaf`g` g`jUzf[bj a`a`9ZheX`%\$!

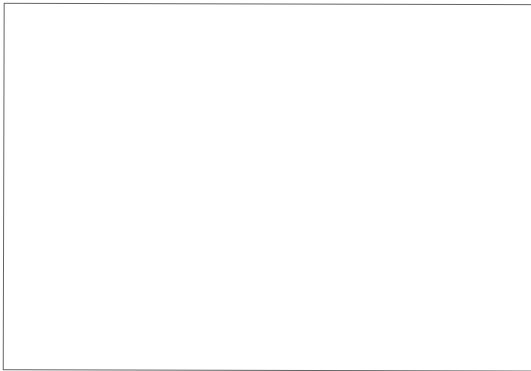


Figure 21: Specifying a user-defined intensity distribution

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.

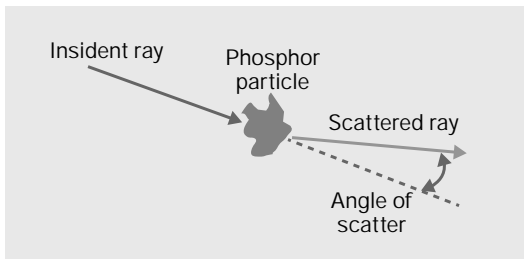


Figure 22: Graphical depiction of the unconverted intensity scatter angle

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 11 for more information. The data in this table can also be loaded from an external file. The format

The last control that must be considered for the phosphor particle is labeled Probabilistic Ray Splii0.0(y Splii0r)8.2 (y Splolle ca254a254a254

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:

10. The absorption spectrum
11. The excitation spectrum/quantum yield
12. The mean free path
13. The emission spectra
14. The refractive index of the phosphor

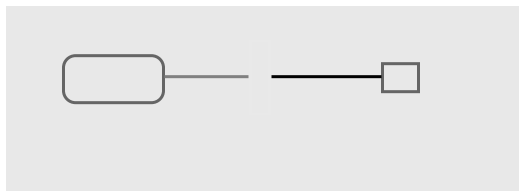
Luckily, the first three inputs can be calculated from a simple inline transmission measurement. This section discusses how to obtain these parameters and how they are applied to various phosphor applications.

Obtaining Inline Transmission

The inline transmission (T_{λ}) is a wavelength-dependent set of values. 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 24.



Equation 14

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

where
 D = Sample Thickness

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

Equation 15

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

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) and the total Fresnel transmission (T_F) shows the relationship between the bulk transmission, the inline transmission, and the total Fresnel transmission (T_i).

Equation 16

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

The total Fresnel transmission is related to the total Fresnel reflectance (R_F) by

Equation 17

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

The total Fresnel reflectance is the reflectance due to the first and second 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).

Equation 18

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

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

Equation 19

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

The contribution to the total Fresnel transmission of the high order reflections is small. Consequently, a good approximation for

Equation 20

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

where

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

Φ_{Em} (given by the absorbed power scaled by the quantum yield value and the Stoke's Shift, is the integrated

Equation 26

$$\Phi_{Em} = OY \cdot \Phi \cdot SS$$

$SS = \text{Stoke's Shift}$

$$SS = \frac{\int_{-\infty}^{\infty} \lambda \cdot Em(\lambda) d\lambda}{Em(\lambda_0)}$$

The total emitted power cannot be obtained directly from the inline transmission measurement. Instead, an integrating sphere and a spectrometer must be used to capture and measure the isotropically-emitted radiation.

relationship for the Stoke's Shift and the weighting used to calculate the emitted wavelength from the emission spectrum.

Equation 27

$$SS = \frac{\lambda_0}{\lambda_1}$$

where

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

relationship for the Stoke's Shift and the weighting used to calculate the emitted wavelength from the emission spectrum.

Equation 28

$$SS = \frac{\lambda_0}{\lambda_1} = \frac{\int_{-\infty}^{\infty} \lambda \cdot Em(\lambda) d\lambda}{\int_{-\infty}^{\infty} Em(\lambda) d\lambda}$$

relationship for the Stoke's Shift and the weighting used to calculate the emitted wavelength from the emission spectrum.

Equation 29

$$\frac{\Phi_{Em}}{\Phi_{Em} + \Phi_{F} + \Phi_{IT}} = \frac{\Phi_{Em}}{\Phi_{Em} + \Phi_{F} + \Phi_{IT}}$$

You might notice that the last addend in Equation (29) is the inline transmission (T). The second to last term is the total Fresnel

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 LightTools".

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,

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

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

Equation 32