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Investigating the Interplay of Absorption and Scattering in Phosphor-Converted LEDs Using a GPU-Accelerated Monte Carlo Framework

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Abstract

Optimizing phosphor-converted light-emitting diodes is challenging due to the complex interplay of absorption, elastic scattering and luminescence. Unlike previous studies that focused on characterizing optical parameters, this work isolates their individual contributions in order to derive fundamental design limits. We present a comprehensive analysis using a GPU-accelerated Monte Carlo framework that solves the luminescent radiative transfer equation, including the full luminescence cascade. We systematically investigate the influence of the absorption (μ_a) and scattering (μ_s) coefficients by varying them over a range of 0.1 to 10 times the reference values of a standard phosphor (0.8 wt%). We found that transmitted luminescence saturates when absorption exceeds approximately three times the reference value ($\mu_a \approx 1.2 \text{ mm}^{-1}$) and peaks at an optimal μ_s before backscattering losses dominate. In high-concentration regimes, mirror-assisted geometries are shown to enhance backward emission by a factor of 2.1 compared to open boundaries. Our findings provide model-based predictions for luminescence transport in phosphor–polymer composites.

Keywords: Monte Carlo simulation; radiative transfer equation; phosphor-converted LEDs; luminescence; fluorescence; optical properties; light propagation; scattering media

1. Introduction

Phosphor-converted light-emitting diodes (pcLEDs), which consist of a blue LED chip combined with one or more phosphor layers, are the most widespread configuration for generating white light [1–4]. In this design, part of the incident blue light is absorbed by the phosphor and re-emitted at longer wavelengths via a down-conversion process, typically yielding a broad emission band in the green-to-red range. Despite their ubiquity, the design and optimization of pcLEDs largely relies on iterative trial-and-error approaches complemented by extensive measurements [1,5,6]. Modeling the optical behavior of phosphor layers is challenging due to the complex interplay between absorption, multiple scattering, and luminescence re-emission. Previous studies have shown that this interplay fundamentally determines the efficiency and color uniformity of pcLEDs [7–9]. Monte Carlo and hybrid ray-tracing approaches have been extensively used in device-level modeling to optimize packaging geometry and efficiency [6,10,11]. These investigations have quantified the impact of particle size [12], concentrations [13–15] and re-absorption [16], determining factors for color and angular homogeneity [17–21].

However, most existing models rely on simplifications, such as isotropic scattering and diffusion theory approximations [7], analytical assumptions that are only valid for



Received: 5 January 2026

Revised: 10 February 2026

Accepted: 17 February 2026

Published: 21 February 2026

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weak absorption regimes [22], or two-wavelength treatments that neglect spectral overlap between excitation and emission [1,23,24].

Recent efforts have begun to address these limitations through spectral and multi-wavelength models of phosphor transport [6,25]. Nevertheless, a unified, quantitative analysis remains limited. A key challenge in experimental optimization is that absorption (μ_a) and scattering (μ_s) coefficients are inherently coupled by the phosphor concentration or particle size. Consequently, it is difficult to isolate the individual contributions of scattering and absorption to loss mechanisms or spatial energy distribution. Therefore, a rigorous simulation approach is necessary to decouple these parameters and identify fundamental design limits.

In our previous work, we focused on the inverse problem: developing and validating wavelength-resolved methods for determining the intrinsic optical properties, quantum yield, and emission probability of luminescent media from integrating sphere measurements [26–28]. While these studies established the accuracy of the underlying Monte Carlo framework for material characterization, they did not explore the forward problem of device optimization.

Our GPU-accelerated framework enables rapid parameter sweeps and detailed analysis of spectral and angular emission distributions. Unlike diffusion-based approximations or two-wavelength models, this framework solves the full luminescent radiative transfer equation (FRTE) without simplifying the spectral cascade, making it uniquely suitable to predict performance limits in regimes where analytical models fail.

In this study, we present a systemic parametric exploration using this previous developed and validated framework to investigate how the optical properties and phosphor concentration, specifically the balance between absorption and multiple scattering, govern the light transport and luminescence efficiency in pcLEDs. By numerically decoupling μ_a and μ_s , we go beyond experimental capabilities to identify characteristic trends, such as luminescence saturation at high absorption and optimal scattering conditions for maximal emission. We also calculate the predicted potential gain from mirror-assisted geometries. The results offer a comprehensive physical understanding of light redistribution within phosphor layers and provide practical guidelines for designing efficient LEDs operating in the linear transport regime. Furthermore, this computational approach allows for rapid, cost-effective, and precise parameter sweeps across extensive configurations, which would otherwise be time-consuming and expensive to achieve experimentally.

2. Method

2.1. Optical Properties

To ensure realistic input parameters for the simulation, we prepared and characterized a physical phosphor sample to determine the intrinsic optical properties. The phosphor used in this study was LP-N620-04-00, supplied by Leuchtstoffwerk Breitung GmbH, Breitung, Germany. To prepare the sample, the phosphor powder was dispersed homogeneously in a polydimethylsiloxane (PDMS) matrix (Elastosil M 4641 A/B, Wacker Chemie AG, Munich, Germany). The optical properties of this phosphor–PDMS composite were determined using a custom-made integrating sphere-based setup [26,27]. For this purpose, the mixture was cast into slabs of approximately 2 mm thickness, resulting in a phosphor concentration of 0.8 wt%. This thickness was chosen to minimize errors when determining the intrinsic optical properties.

The use of the integrating sphere-based setup yields the optical properties of both phosphor and matrix: wavelength-dependent absorption $\mu_a(\lambda)$ and scattering $\mu_s(\lambda)$ coefficients. At 420 nm, near the absorption maximum, the absorption coefficient was found to be $\mu_a(420\text{ nm}) \approx 0.4\text{ mm}^{-1}$ and the reduced scattering coefficient $\mu'_s(\lambda) \approx 0.6\text{ mm}^{-1}$.

The PDMS matrix contributes negligibly to scattering and exhibits a weak wavelength-dependent absorption of $\mu_a \approx 0.03 \text{ mm}^{-1}$ and a refractive index of $n(\lambda) \approx 1.4$. The phase function was modeled using the Henyey–Greenstein distribution with an anisotropy factor $g = 0.78$, which is representative for commercial phosphor–PDMS composites [29]. The anisotropy factor was assumed to be wavelength-independent, consistent with previous studies on similar materials [7,25]. This assumption is justified because the phosphor consists of particles with a mean diameter of $d_{50} = 7 \text{ }\mu\text{m}$, placing them well within the Mie regime, where the particle size exceeds the optical wavelength by an order of magnitude. Additionally, the refractive index mismatch between the phosphor and the surrounding matrix does not change a lot versus wavelength. Multiple scattering effects mask the influence of any small decrease in g at longer wavelengths. The intrinsic quantum yield and emission probability distribution were obtained following the method described in [28]. The intrinsic quantum yield was close to 1. Thermal quenching and temperature-dependent effects were excluded to isolate the impact of optical transport phenomena. To investigate the influence of absorption and scattering separately, the optical properties were changed independently and linearly. A change in both μ_s and μ_a represents a change in phosphor concentration. Although μ_s and μ_a are strongly correlated in real phosphor composites due to particle size and packing density, this theoretical decoupling enables us to isolate the impact of each transport parameter. The scaling factors, which range from 0.1 to 10, were chosen to cover the transition from the ballistic to the diffusive regime and to encompass the typical parameter space of commercial phosphor materials.

2.2. Monte Carlo Simulation Framework

Light transport and luminescence generation were simulated using a GPU-accelerated Monte Carlo framework that we developed very recently [28]. This framework solved the full luminescent radiative transfer equation. The algorithm accounted for wavelength-dependent absorption, scattering and re-emission, treating luminescent and non-luminescent components independently. The wavelength of each photon was sampled from the excitation spectrum. It then propagated through the medium until it was either absorbed, re-emitted, or scattered, or until it exited the geometry. Absorption events were probabilistically assigned to luminescent or non-luminescent components based on the relative absorption coefficients. If absorption occurred in a luminescent component, re-emission was determined by the quantum yield Φ_f and the normalized emission probability distribution $P_f(\lambda)$. Re-emitted photons were assigned a new wavelength λ and isotropic direction. To ensure energy conservation during the Stokes shift (where the photon energy $E \propto 1/\lambda$ decreases), the photon weight is continually updated at each emission event according to [28,30]

$$w_\lambda = w_{\lambda'} \left(\frac{\lambda'}{\lambda} \right), \quad (1)$$

where $w_{\lambda'}$ and λ' denoted the photon's weight and wavelength prior to emission, and w_λ and λ after emission. Photons could undergo multiple cycles of re-absorption and re-emission, enabling the full simulation of the luminescence cascade. Scattering was modeled using the Henyey–Greenstein phase function, and the scattering contribution of the PDMS matrix was neglected relative to the phosphor particles. The GPU kernel was implemented in OpenCL, with host-side control, preprocessing, and postprocessing in Python (version 3.13) and ISO C++ 14-Standard. All simulations were performed on a workstation equipped with an AMD Ryzen 9 7900X CPU (12 cores, 4.7 GHz) and an NVIDIA GeForce RTX 4070 Ti GPU. To allow comparison between an idealized laboratory excitation and a realistic pcLED configuration, two types of excitation sources with a beam diameter of 5 mm were simulated: a collimated beam incident at 8° to the surface normal,

corresponding to the experimental setup [26] and a cosine-weighted diffuse source emitting into the half-space, representing LED emission.

2.3. Detection and Fluence Evaluation

The photons exiting the slab geometry were categorized by tracking their interaction history and exit boundary. During propagation, each photon was flagged whether it remained an excitation photon or was converted into a luminescence photon. After exciting the simulation volume, their direction was evaluated relative to the incident light. Those that left the medium in the forward direction (opposite to the source) were classified as transmission (T) and photons backscattered through the entrance plane were classified as reflection (R). The accumulated counts of excitation and luminescence photons in both directions were normalized by the total initial photon count. To evaluate angular emission profiles, the exit direction of each photon was transformed to spherical coordinates (θ, ϕ) . The polar angle $\theta \in [0, \pi]$ was discretized into bins of $\Delta\theta = 1^\circ$, while full integration over ϕ yielded an axially symmetric distribution. Each bin was normalized by the corresponding solid angle

$$\Delta\Omega_i = 2\pi \left[\cos\left(\theta_i - \frac{\Delta\theta}{2}\right) - \cos\left(\theta_i + \frac{\Delta\theta}{2}\right) \right], \quad (2)$$

and by the total number of launched photons N_0 .

The volumetric fluence $\Phi(x, y, z)$ within the medium was computed using a Cartesian voxel grid with cell sizes Δx , Δy , and Δz . At each scattering step, the photon's contribution to the local fluence was estimated using a scattering-based collision estimator. The local contribution, $\Delta\Phi$, was calculated as

$$\Delta\Phi = \frac{w}{\mu_s(\lambda)}, \quad (3)$$

where w represents the current photon weight and $\mu_s(\lambda)$ represents the wavelength-dependent scattering coefficient. The total local fluence in each voxel was then obtained by summing over all photon steps n within that voxel, for either the excitation or luminescence field, depending on the photon's current state. The total accumulated value in each voxel is normalized by the voxel volume and the number of launched photons to yield the fluence. An input power of $P_{\text{in}} = 1$ W was assumed. Because the Monte Carlo method is linear, the presented results can be arbitrarily scaled to other power levels.

We validated the Monte Carlo implementation and luminescence weighting scheme using our previously published digital optical twin of the integrating sphere setup and this was then benchmarked against experimental data [28].

3. Results

The following sections analyze the impact of optical properties on the efficiency and light distribution of pcLEDs. To prioritize physical interpretation, we present selected data that best demonstrate behaviors such as saturation effects and optimal scattering regimes. A comprehensive atlas of the complete simulation dataset, including full spectral data, sensitivity analyses, and comparative fluence maps for collimated and diffuse excitation sources, is provided in the Supplementary Information (Figures S1–S13).

3.1. Influence of the Absorption Coefficient μ_a on Luminescence

For efficient light conversion in phosphor layers, the phosphor particles must absorb the excitation photons. Therefore, an increase in the absorption coefficient μ_a initially increases the amount of light converted into luminescence. The absorption measured at 0.8 wt% serves as the reference value for μ_a . To isolate this effect, this reference value was scaled by a factor ranging from 0.1 to 10, while the scattering coefficient was kept constant.

Figure 1a shows that the transmitted luminescence increases with μ_a until it saturates at 3.3 times the reference absorption (corresponding to approximately 2.64 wt%, assuming a linear relationship between concentration and absorption). Beyond this point, further increases in μ_a no longer improve the transmitted luminescence yield, but instead lead to a slight decline, whereas reflected luminescence continues to rise. Ideally, the total residual excitation, defined as the sum of the transmitted and reflected excitation fractions ($T_{\text{ex}} + R_{\text{ex}}$), should be minimized to ensure maximal conversion. The sensitivity analysis, defined as the change in the fraction of input photons F with respect to absorption coefficient ($\Delta F / \Delta \mu_a$, see Figure S1b), demonstrates that the response is strongest for small μ_a , indicating that small changes in absorption have a large impact when the excitation light still penetrates deeply into the phosphor layer. In contrast, at high μ_a , the excitation is mostly absorbed near the surface, as illustrated by the fluence distributions in Figure 1c,d, which depict the LED light source case. This surface confinement prevents generated luminescence from escaping in transmission and increases reabsorption losses. Moreover, the high absorption density creates a substantial thermal load close to the chip surface, increasing the risk of thermal quenching. This behavior indicates a shift from an excitation-limited regime, where moderate absorption is advantageous for ensuring complete excitation conversion, to an emission-limited one, where excessive absorption becomes counterproductive. These findings align with the trade-off between excitation efficiency and reabsorption losses reported in earlier studies [31–33]. Comprehensive datasets supporting this analysis of the variation of μ_a (Figure S1), as well as a comparison of the fluence distributions for the collimated source (Figure S2) and the LED source (Figure S3) at varying concentrations, are provided in the Supplementary Information.

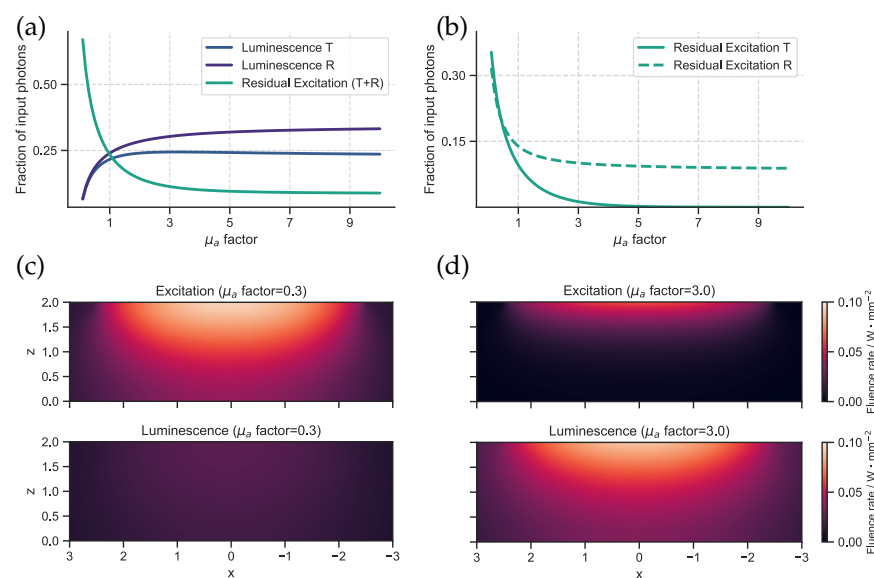


Figure 1. Simulation of absorption coefficient variation. (a) Fraction of input photons converted to luminescence (transmission T, reflection R) and the total residual excitation as a function of the μ_a scaling factor. (b) Breakdown of the residual excitation into transmitted and reflected components. (c,d) Spatial distributions of the normalized fluence $\Phi(x, z)$ for μ_a scaling factors of 0.3 and 3.0, respectively. The top panels display the excitation field, while the bottom panels show the generated luminescence.

3.2. Effect of the Scattering Coefficient μ_s and Optimal Scattering Regime

Scattering of the phosphor strongly impacts the probability that emitted luminescence photons can escape the layer [12]. To investigate this phenomenon, the absorption coefficient was kept constant while varying only the scattering coefficient μ_s in the simulation. As Figure 2a shows, luminescence remains weak at very low μ_s , because the excitation light propagates nearly ballistically, interacting with few phosphor particles. Moderate

scattering improves the excitation distribution throughout the volume, increasing the probability of absorption and subsequent re-emission. However, as μ_s increases further, this trend reverses. Strong multiple scattering limits the optical penetration depth and enhances backward scattering. For scattering coefficients above the optimal range, the residual excitation reflected from the entrance surface rises steadily (Figure 2b), accompanied by a strong 420 nm excitation peak and a higher luminescence yield in reflection (Figure 2c). In transmission, however, Figure 2d shows a drop in luminescence for higher μ_s . Although the residual excitation light is reduced, this should not be misinterpreted as a higher conversion rate. The dominant backscattering reduces the transmitted luminescence. Based on our systematic parameter sweep, the model predicts a distinct maximum at 0.8 times the reference scattering in transmission that defines the optimal scattering regime for forward-emitting pcLEDs.

This maximum varies based on the phosphor's scattering properties [34]. Several experimental works have reported similar conclusions. By reducing scattering through refractive index matching or using weakly scattering large phosphor particles, the overall efficiency can be increased [35–38]. Our simulations confirm that, while a certain degree of scattering is required for excitation homogenization, excessive scattering causes light trapping and reabsorption losses. From a practical perspective, achieving this optimal regime requires adjusting the particle size distribution and the refractive index contrast. Larger phosphors are generally preferable, because they have a lower scattering coefficient at the same weight concentration. Additionally, minimizing the refractive index mismatch reduces the scattering strength and shifts the system away from the loss-dominated, high- μ_s regime. Designers should therefore aim for a balance by selecting particles that scatter just enough to ensure angular color homogeneity without surpassing the optimal scattering threshold. Extended datasets supporting these conclusions, including fluence distribution comparisons for collimated and LED sources, are provided in the Supplementary Information (Figures S4–S6).

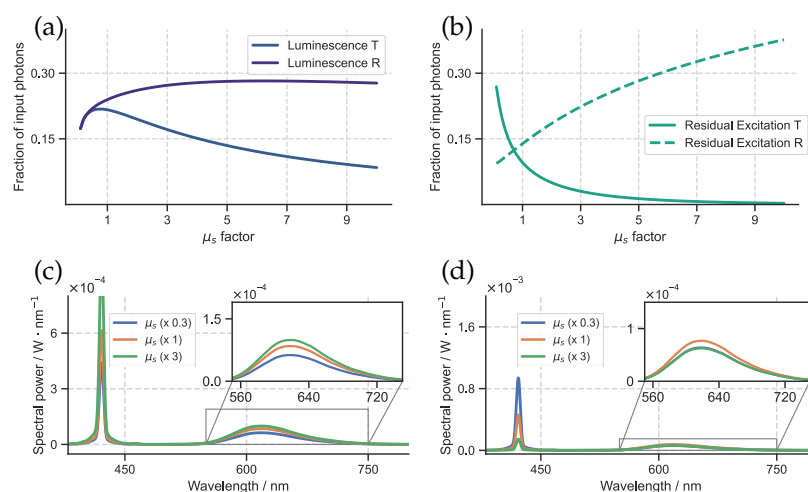


Figure 2. Simulation of scattering coefficient variation. (a) Luminescence as a function of μ_s factor. (b) Excitation as a function of μ_s factor. (c) Resulting spectra for different μ_s scaling factors in reflection. (d) Resulting spectra for different μ_s scaling factors in transmission.

3.3. Effect of Phosphor Concentration: Simultaneous Increase in μ_a and μ_s

In practical phosphor composites, increasing the concentration of phosphors simultaneously raises μ_a and μ_s , because the absorption and scattering are dominated by the particles rather than the encapsulation matrix. As a result, the overall behavior represents a superposition of the individual trends observed in the previous sections: enhanced conversion efficiency from higher absorption and increased light redistribution from stronger

scattering. In practice, the ratio of the scattering and absorption coefficients is largely determined by the particle size distribution of the phosphor [39,40]. Therefore, adjusting the particle size, by grinding or selecting specific fractions, offers a direct process parameter to tune the μ_s/μ_a ratio towards the ideal operating point identified in our simulations. At low concentrations, both μ_a and μ_s remain small. The excitation light therefore penetrates deeply into the phosphor layer. As visualized in the fluence maps in Supplementary Figures S7 and S8, only a fraction of this light is absorbed. While luminescence generation occurs throughout the volume, the absolute output is limited by the insufficient absorption probability. As the concentration increases, μ_a rises, leading to more efficient excitation-to-luminescence conversion and a rapid increase in total luminescence emission. At the same time, moderate values of μ_s improve the spatial distribution of the excitation within the layer, allowing photons to interact with more phosphor particles and further increasing the luminescence yield. This constructive combination of both effects drives the strong initial rise in transmitted luminescence shown in Figure 3a.

However, beyond this optimal regime, both coefficients become large enough to introduce cumulative loss mechanisms. As shown in the fluence distributions in Figure S8, the excitation field shifts from deep penetration at low concentrations to strong confinement within a thin, near-surface layer at high concentrations. This surface confinement, combined with high scattering, creates a barrier for forward propagation. Consequently, the transmitted luminescence saturates and eventually declines as the effective penetration depth becomes significantly smaller than the layer thickness. In contrast, the reflected luminescence continues to rise. Due to the isotropic nature of the emission, a large fraction of the generated luminescence near the surface immediately propagate backward. This effect is amplified by the high scattering coefficient, which effectively redirects potential forward-propagating photons back towards the entrance. This saturation behavior mirrors experimental findings [31]. These authors observed a similar saturation of the re-emitted flux above phosphor densities of 3–5 wt%. It is important to note that, while these trends are universal, the absolute concentration values scale with geometry. This requires a corresponding change in phosphor concentration when changing the slab thickness to maintain the same optical depth. In high-density regimes, non-linear effects such as quenching of luminescence due to high concentrations and dependent scattering, which are not included in this linear transport model, could become limiting factors. Nevertheless, from the standpoint of optical transport, backscattering remains the dominant limitation on transmission efficiency. Consequently, it becomes advantageous to either utilize this backward-propagating fraction directly in reflection geometry or redirect it using reflective cups and back-surface mirrors to improve overall efficiency [5,35].

3.4. Effect of Illumination Angle and Reflective Geometry

In conventional pcLEDs, the phosphor layer is typically placed directly on or above the die [4,41]. This leads to a transmission geometry where backward-propagating light is partially reflected, but also significantly absorbed by the chip and package, representing a significant loss factor. As our simulations in Section 3.3 show (Figure 3), reflected luminescence becomes the dominant component at high phosphor concentrations, making it more important to recover this light. Alternative designs have been proposed to address these limitations: remote-phosphor configurations primarily mitigate thermal issues by decoupling the phosphor layer from the heat source, while reflective geometries focus on maximizing light extraction [5,35,36,42].

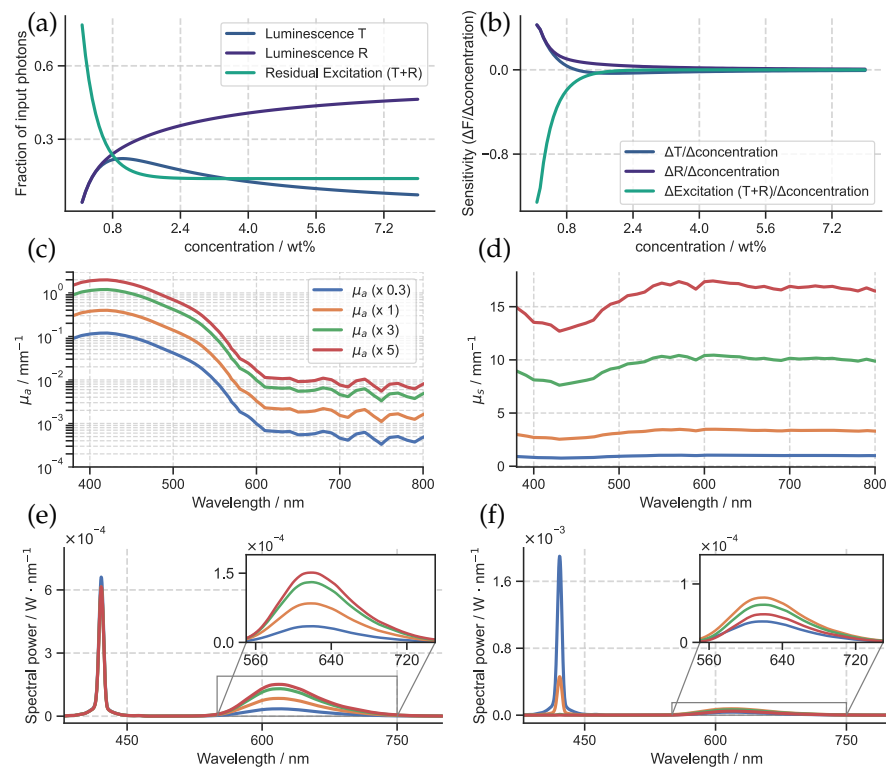


Figure 3. (a) Luminescence (transmission T, reflection R) and total residual excitation as a function of concentration. (b) Sensitivity analysis, showing the change in the fraction of input photons ΔF with change in concentration. This is shown for transmitted luminescence ΔT , reflected luminescence ΔR , and total residual excitation $\Delta \text{Excitation (T+R)}$. (c,d) Wavelength-dependent input parameters for absorption coefficient $\mu_a(\lambda)$ and scattering coefficient $\mu_s(\lambda)$. A scaling factor of 1.0 corresponds to a concentration of 0.8 wt% (orange). Comparative concentrations are color-coded: 0.24 wt% (blue), 2.4 wt% (green), and 4.0 wt% (red). (e,f) Simulated spectra for reflection and transmission, respectively.

Motivated by these concepts, we investigated the potential of such reflective geometries under varying illumination angles α (defined in Figure 4a). We first analyzed the dependence of the luminescence with respect to the incident angle. Most LEDs emit approximately as Lambertian sources, with intensity following $I(\theta) \propto \cos(\theta)$. However, some real devices can deviate from this pattern and can be approximated as the sum of different Gaussians or cosine-power functions [43]. The simulation results, detailed in the Supplementary Information (Figures S9 and S10), revealed that for a collimated beam, the total luminescence yield in reflection remained robust and nearly constant for incident angles ranging from normal incidence (90°) down to 20° . A significant drop in yield was observed only at grazing angles below 20° .

To quantify the potential for light recycling, we then simulated a “mirror-assisted” geometry by introducing a reflective back surface behind the phosphor layer (Figure 4b). The back surface was modeled as a physical silver mirror with complex refractive index values ($n = 0.05, k = 3.9$), resulting in a realistic reflectivity of $R \approx 98.3\%$. As shown in Figure 4c,d, the addition of this mirror effectively redirects light that would otherwise be lost through transmission. The backward detected luminescence is enhanced by a factor of more than two.

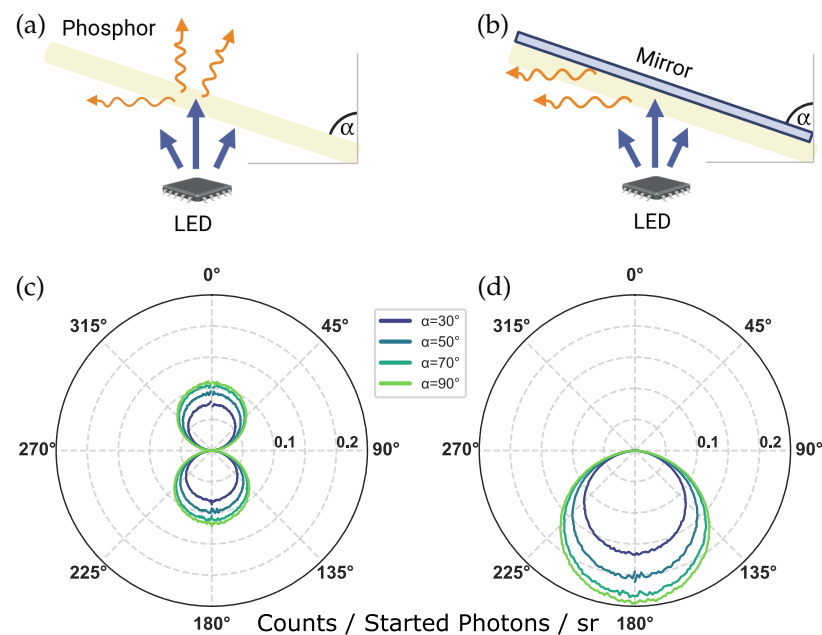


Figure 4. Comparison of standard and mirror-assisted geometries under varying incident angles α . (a) Schematic of the standard phosphor layer geometry, defining α as the angle between the excitation beam (blue arrows) and the phosphor surface. Orange arrows indicate the re-emitted light. (b) Schematic of the mirror-assisted geometry with a reflective back surface. (c,d) Angular luminescence distribution visualized as polar plots. The upper hemisphere (270° – 90°) corresponds to transmission (forward direction), while the lower hemisphere (90° – 270°) corresponds to reflection (backward direction) (c) Standard geometry showing emission in both directions. (d) Mirror-assisted geometry showing a significant increase in reflection due to the redirection of transmitted light.

In addition to improving photon recycling, reflective geometries combined with oblique incidence can more uniformly spread the absorption region, as indicated by the fluence distributions in Figures S12 and S13. Since the local heat generation is directly proportional to the absorbed excitation energy density, this spatial homogenization helps to mitigate local hotspots near the entrance plane. This is particularly critical at high irradiance, where material saturation and thermal quenching are relevant issues [44]. Although considerations for building such a source have been made in the past [42,45], the design has received less attention than transmission geometries. This could open up opportunities for more efficient pcLEDs. Although this study uses a planar mirror to illustrate the increase in extraction efficiency, practical applications frequently necessitate directional beam shaping. The broad, Lambertian-like emission profile observed in the reflection geometry (Figure 4d) is ideal for secondary optics, such as parabolic or concave reflectors. This is particularly relevant for high-luminance applications, such as automotive headlamps, unmanned aerial vehicle (UAV) lighting, and high-intensity flashlights, where the total optical throughput is limited by source efficiency.

3.5. Physical Validity and High-Power Limitations

It is important to contextualize these results within the fundamental assumptions of the RTE. Our framework solves the RTE in the linear regime by treating the quantum yield as constant and intrinsic material property. However, in real-world device operation, non-linear mechanisms, can act as additional loss channels or alter optical properties. Therefore, the efficiency values and optimal geometries identified in this work effectively serve as a robust baseline determined by photon transport and linear material characteristics. In high-power applications, ground-state depletion and thermal quenching become critical at high irradiances. While mid-power LEDs typically operate at irradiances below 0.5 W/mm^2 ,

automotive high-power LEDs reach densities of 2–5 W/mm², and laser-driven lighting can exceed 10 W/mm² [46,47]. For the parameters used in this study (1 W distributed over a 5 mm spot), the resulting irradiance is approximately 0.05 W/mm². This value is orders of magnitude below the saturation threshold $I_{10\%}$ (irradiance causing a 10% efficiency drop), which is reported at ≈ 1.4 W/mm² for red nitride phosphors and up to 7.5 W/mm² for YAG:Ce [44,48,49]. Regarding particle density, the assumption of independent scattering should remain valid for the investigated phosphor loads. We simulated concentrations up to 8 wt%, which corresponds to a volume fraction of approximately 2 vol%. This is significantly below the thresholds, where dependent scattering and near-field coupling should have an influence (typically > 10 vol%) [50–52]. Similarly, inter-particle concentration quenching is negligible at these low volume fractions [48]. Further sensitivity checks revealed that changing the anisotropy factor g from 0.5 to values approaching 1.0 alters the total transmitted luminescence yield by less than 0.9 percentage points. While our results characterize the efficiency in the absence of non-linear losses, the low-excitation investigated here ensures that these linear predictions are close approximations of realistic device performance for general lighting and remote-phosphor applications. For ultra-high-luminance architectures, however, the effective quantum yield would likely decrease due to the aforementioned saturation effects, necessitating a correction of the optima towards lower phosphor loads or larger spot sizes. Although the underlying physical framework has been rigorously validated through material characterization [26–28], applying it to specific pcLED geometries depends on the transitivity of the radiative transfer model. We acknowledge that full device-level performance is influenced by package-specific boundary conditions, such as chip-level self-absorption and additional optics. However, these conditions are not the focus of this study. Therefore, the quantitative trends identified here establish a theoretical baseline, and comprehensive device-level benchmarking is a goal for future work.

4. Conclusions

The quantitative findings presented in this study, including the identified μ_s saturation points and mirror-assisted gain factors, are intended as model-based predictions under the conditions investigated. We used an established, validated spectral Monte Carlo framework to simulate luminescence transport in phosphor–polymer composites and conduct a thorough parametric analysis of phosphor layers in pcLEDs.

Our simulations identify three characteristic design regimes.

First, increasing absorption enhances excitation–luminescence conversion only until a maximum is reached. Beyond moderate values, excitation becomes confined near the entrance surface, and reabsorption suppresses forward extraction. For the specific phosphor system investigated, this physical limit manifests as a saturation threshold at a concentration of 2.64 wt%, with scaling factor of 3.3.

Second, scattering plays a dual role. Moderate scattering homogenizes excitation and enhances emission yield. Excessive multiple scattering, on the other hand, increases backscattering and reduces transmission. This defines an optimal scattering window for transmission-based pcLEDs, observed here at 0.8 times the reference scattering level. Consequently, optimization in practice requires tuning the μ_s/μ_a ratio, for example, through the selection of suitable particle sizes, in order to match this window.

Third, when absorption and scattering increase simultaneously, as occurs with higher phosphor concentrations, their effects combine. Transmitted luminescence exhibits a pronounced maximum followed by a decline, while reflected luminescence continues to rise due to near-surface excitation confinement. Mirror-assisted and remote-phosphor geometries could partially recover luminescence that would otherwise be lost to backscattering. Our simulations showed that such photon-recycling designs can more than double the

reflection signal. This suggests that for high-concentration phosphors, geometric optimization (e.g., mirrors) is more effective than material optimization alone. However, the current model disregards non-linear phenomena relevant under high irradiance, such as absorption saturation (ground-state depletion) and thermal quenching. Future work could integrate thermal coupling and concentration quenching models to refine the optimization of high-power devices.

Supplementary Materials: The following supporting information can be downloaded at: <https://www.mdpi.com/article/10.3390/photonics13020206/s1>, Figure S1: Impact of the absorption coefficient μ_a on luminescence efficiency, sensitivity, and emission spectra; Figure S2: Fluence rate distribution $\Phi(x, z)$ for varying μ_a under collimated illumination (e.g., laser); Figure S3: Fluence rate distribution $\Phi(x, z)$ for varying μ_a under diffuse LED illumination (cosine distribution); Figure S4: Impact of the scattering coefficient μ_s on luminescence efficiency, sensitivity, and emission spectra; Figure S5: Fluence rate distribution $\Phi(x, z)$ for varying μ_s with a collimated light source; Figure S6: Fluence rate distribution $\Phi(x, z)$ for varying μ_s with an LED source; Figure S7: Fluence rate distribution $\Phi(x, z)$ for different phosphor concentrations under collimated illumination; Figure S8: Fluence rate distribution $\Phi(x, z)$ for different phosphor concentrations under LED illumination (cosine distribution); Figure S9: Simulation results for different incident angles with a collimated light source (e.g., laser) for a standard phosphor layer geometry (non-mirrored); Figure S10: Impact of incident angle α on luminescence efficiency and emission spectra (diffuse LED source); Figure S11: Simulation results for different incident angles α , with a collimated light source (e.g., laser) for a phosphor layer with a mirror; Figure S12: Fluence rate distribution $\Phi(x, z)$ for different incident angles α (LED source, no mirror); Figure S13: Fluence rate distribution $\Phi(x, z)$ for different incident angles α in a mirror-assisted setup (LED source).

Author Contributions: Conceptualization, P.G., J.J. and F.F.; methodology, P.G.; software, P.G. and F.F.; validation, P.G., J.J. and F.F.; formal analysis, P.G.; investigation, P.G.; resources, A.K.; data curation, P.G.; writing—original draft preparation, P.G.; writing—review and editing, P.G., J.J., F.F. and A.K.; visualization, P.G.; supervision, A.K. and F.F.; project administration, A.K.; funding acquisition, A.K. All authors have read and agreed to the published version of the manuscript.

Funding: This research was funded by Invest BW (VDI/VDE Innovation + Technik GmbH) within the project AdelPhos (BW1-5125/0). This research is part of the Zentrum zur Bestimmung der optischen Eigenschaften (ZOE, Center of the Determination of Optical Properties of Scattering Media) at the ILM Ulm.

Data Availability Statement: The data that support the findings of this study are available from the corresponding author, P.G., upon reasonable request due to privacy.

Acknowledgments: We thank David Hevisov and Dominik Reitzle for fruitful discussions and helpful suggestions throughout the project.

Conflicts of Interest: The authors declare that this study received funding from Invest BW (VDI/VDE Innovation + Technik GmbH). The funder was not involved in the study design, collection, analysis, interpretation of data, the writing of this article or the decision to submit it for publication.

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