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MONTE CARLO RAY-TRACING SIMULATION

FOR OPTIMIZING LUMINESCENT SOLAR CONCENTRATORS

A Thesis in

Engineering Science

by

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ABSTRACT

Luminescent solar concentrators (LSCs) use fluorescent materials embedded in an optical waveguide to absorb, reemit, and concentrate incident solar irradiance to the edges of the waveguide. Photovoltaic (PV) cells attached to the edges of an LSC can harvest the concentrated irradiance and reduce the cost of harvesting solar power. A robust and user-friendly Monte Carlo ray-tracing simulation was developed for this thesis to study the efficiencies, loss mechanisms, and costs of LSC systems employing a wide variety of different fluorescent materials and PV cells. Specifically, the simulation software was used to study the performance of infrared emitting PbSe quantum dot LSCs, estimate the efficiencies of non-conventional PV cells in LSC designs, assess the present capabilities of conventional LSC systems to harvest solar power at reduced cost, and investigate the viability of building-integrated LSC systems.

Infrared emitting PbSe QD LSCs that employed Ge PV cells were found to suffer from severe self-absorption and down conversion losses, resulting in relatively poor device performance. The power conversion efficiencies of simulated PbSe QD LSCs in AM1.5 solar illumination were estimated to be on the order of 1%, with flux concentration factors of about 4. Tandem PbSe QD LSC layers were found to improve the net power conversion efficiency of visible-harvesting LSC systems employing Si PV cells by 10 to 20%. However, greater efficiency enhancement can be obtained by simply adding a back-surface reflector to the visible harvesting LSC.

Simulation results suggest that LSC systems employing CdTe and organic PV cells will perform very well due to their low cost, high voltage output, and high quantum efficiency within the emission spectrum of Red305, which is a high efficiency organic dye commonly used in LSC research. Cost optimization studies of simulated LSCs suggest that optimal LSC thickness is very thin, on the order of 1mm or less regardless of the chosen material system. Due to the fact that cost-optimized LSC designs were obtained at very thin dimensions, and the use of back-surface reflectors can further reduce cost and improve efficiency, a new idea was proposed in this research to use thin, high aspect ratio LSCs with back-surface reflectors as solar harvesting window blinds and shutters for building-integrated LSC applications. Both window and window blind LSC configurations can effectively reduce the cost of harvesting solar power to less than $1/W, but power conversion efficiencies are limited to about 3 or 4% with presently available fluorescent materials and PV cells. Tandem LSC systems can be used in place of double or triple-pane windows to improve the power conversion efficiency of LSC systems without significantly increasing effective cost, but more research needs to be done to find optimal, high-efficiency fluorescent materials with relatively non-overlapping absorption spectra to improve the efficiency of tandem LSC systems.

Although LSCs are capable of reducing the cost-per-watt of harvesting solar power, their efficiency is still too low to be competitive with conventional PV technology. The future outlook and commercial viability of LSC systems beyond niche application is dependent upon the development of improved waveguide structures and/or highly efficient, non-self-absorbing fluorescent materials.
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Chapter 1: Introduction

1.1 – Luminescent Solar Concentrators

A luminescent solar concentrator (LSC), also known as a fluorescence solar concentrator (FSC), is a device used to absorb, reemit, and concentrate solar power to the edges of a planar waveguide via the total-internal-reflection (TIR) of photons emitted by fluorescent particles embedded within the waveguide [1], [2]. Photovoltaic (PV) cells attached to the edges of the LSC are used to convert collected photons into usable electrical power. Figure 1 shows a schematic illustration of an LSC employing a blue-emitting fluorescent material with a partial exploded view of the attached PV cells.

![Illustration of a luminescent solar concentrator employing a blue-emitting fluorescent material with an exploded view of the attached photovoltaic cells. Absorbed sunlight causes fluorescence emission that can be trapped in the waveguide due to total-internal-reflection.](image)

The system can be imagined as a simple panel of glass or plastic doped with fluorescent particles. Given that solar cells are generally expensive [3] and typical waveguide materials [4] and fluorescent materials [5] are relatively cheap, LSCs can reduce the cost of harvesting solar power by concentrating sunlight and reducing the necessary area of PV cells. In addition, LSCs are efficient collectors of diffuse light, thereby enabling efficient energy conversion during overcast weather conditions and eliminating the need for expensive solar tracking devices [6], [7]. Furthermore, LSCs can be used for building integrated photovoltaics (BIPV) whereby photovoltaic systems can be installed directly into architecture to reduce installation costs [8]. For example, LSCs can act in place of windows in traditional architecture while still maintaining their solar...
power harvesting capabilities. Figure 2 shows a photograph of four LSCs developed at MIT that utilize red, yellow, green, and blue emitting fluorescent dyes [9].

![Image of LSCs](image)

**Figure 2:** LSCs embedded with red, yellow, green, and blue emitting organic dyes [9].
(Photo by Donna Coveney, MIT)

The idea of using fluorescent particles embedded in a waveguide to concentrate light was originally proposed in the late 1970’s by Weber and Lambe [1]. Rapid progress was made in the first decade of LSC development, but advances soon slowed due to a lack of fluorescent materials with suitable characteristics such as long-term photostability, broad absorption spectra, and minimal absorption/emission spectrum overlap. Most organic laser dyes used in early LSC research only had an active lifespan between a few weeks and a few years [10]. In comparison, conventional solid-state solar cells have a life-span on the order of 30 years [8]. Due to the small 100 – 300nm wide absorption spectra of organic dyes used in the past, it was difficult to absorb a significant portion of the solar spectrum. Additionally, dyes suffered from considerable self-absorption losses due to absorption and emission spectrum overlap [11].

By the early 1980’s, research interest in LSCs began to fade due to lack of progress and unsuitable fluorescent materials. However, LSC research was brought to light once again in the early 2000’s due to the inception of new classes of fluorescent materials and significant improvements made in producing photo-stable organic dyes with high quantum yields [12]. Although photo-stable dyes with reasonably broad absorption spectra have been discovered, self-absorption is a persisting problem that plagues LSC research even today [13]. Rare-earth complexes with strong UV absorption are the only known, usable fluorescent materials to exhibit nearly zero self-absorption loss [14], [15]. However, the absorption spectrum of rare-earth complexes tends to overlap poorly with the solar spectrum.
1.2 – LSC Design

The efficiency of an LSC is dependent on the light trapping capability of the waveguide, the optical properties of the fluorescent material, and the power conversion efficiency of the attached PV cells at the fluorescent material emission wavelengths.

1.2.1 – Waveguide

The waveguide of an LSC should optimally have the following characteristics: high transparency throughout the visible spectrum, nearly perfect transparency at wavelengths within the emission spectrum of the fluorescent material, an index of refraction greater than or equal to 1.5, good photo-stability and durability to achieve a life-span longer than 10 years, and low cost. Additionally, the waveguide material must be able to act as a suitable host matrix for the fluorescent material. Since typical waveguide materials, such as glass and PMMA, have similar light trapping capabilities due to their similar refractive indices near 1.5, a more direct focus is typically placed on finding, studying, and improving fluorescent materials that couple well to available PV cells to improve LSC efficiency. However, recent research efforts are also focusing on designing new types of LSC waveguide structures such as cylindrical LSCs [16], [17], slot waveguide structures [18], and ancillary layers such as wavelength selective filters [19] and patterned thin films [20] that trap and collect light more effectively than conventional LSC waveguides.

1.2.2 – Fluorescent Material

Fluorescent materials are one of the most important components of a conventional LSC design. The fraction sunlight capable of being absorbed and the life-span of an LSC device are almost entirely dependent upon the fluorescent material(s) embedded in the waveguide. The only optical mechanism that is not directly dependent on the fluorescent material is the process of light entrapment, which is dictated primarily by the index of refraction of the waveguide material unless the fluorescent material is designed to have highly directionalized emission. An optimal fluorescent material for LSC development should have a broad absorption spectrum to absorb as much incident solar energy as possible, a narrow emission spectrum couplable to the peak spectral response common PV absorber materials to maximize power conversion efficiency, a significant wavelength shift between absorption and emission to reduce the prevalence of photoluminescence (PL) self-absorption, a high fluorescence quantum yield to ensure high emission probability, stability and resistance to photo-degradation to maximize life-span, and low cost to minimize the cost-per-watt of generating electrical power. If a fluorescent material or combination of fluorescent materials cannot attain these characteristics, LSCs in their present form will ultimately fail [12].
Presently studied fluorescent materials are typically separated into three categories: organic dyes, rare-earth complexes, and quantum dot nanocrystals. The following subsections discuss the three primary types of fluorescent materials currently used in LSC development and the primary advantages and disadvantages of each material relative to the others.

1.2.2.1 – Organic Dyes

Organic dyes were the first and still the most popular type of fluorescent material studied in LSC research. The first types of organic dyes used in early LSC development consisted of organic laser dyes, such as rhodamines, coumarins, and DCM, due to their near-unity fluorescence quantum yields and low cost. The problems associated with organic laser dyes include narrow absorption spectra, short life-spans typically less than a year if exposed to solar irradiance, and moderate absorption/emission spectrum overlap [10], [11]. These problems led researchers to seek out new types of organic dyes and other classes of fluorescent materials that solve one or more of these detrimental problems to improve the efficiencies of LSC devices.

Organic dyes used in LSCs have greatly improved since the 1970’s and 1980’s, especially with the development of perylene based Lumogen® F series dyes commonly used in LSC research due to their improved photostability and life span greater than 5 years, excellent fluorescence quantum yields above 0.90, and a wide variety dye colors [21]. Organic dyes are advantageous compared to rare-earth metals and QDs in some respects due to their extremely high fluorescence quantum yield, low cost, and availability. However, they are disadvantageous in general due to their relatively narrow absorption spectra, relatively broad emission spectra, and absorption/emission spectrum overlap. It is important to note that no extraordinary substitute for organic dyes has been found with equivalently high fluorescence quantum yield and low cost. Furthermore, the highest LSC efficiencies to date have been achieved using organic dyes [22].

1.2.2.2 – Rare-Earth Metals

Rare-earth metals and rare-earth complexes are a class of inorganic fluorescent material, usually comprised of Neodymium (Nd), Europium, and/or Ytterbium (Yb). Some of these fluorescent materials show great promise in LSCs due to their unusual characteristic of having non-overlapping absorption and emission spectra [14], [15]. They also tend to have high fluorescence quantum yields when placed in a suitable host matrix at suitable concentrations. However, the absorptivity of rare-earth complexes tends to be relatively weak and their absorption spectra tends to overlap poorly with the solar spectrum. If a rare-earth complex is produced with a broad absorption spectrum that does not overlap with its emission spectrum, while maintaining high absorptivity, high fluorescence quantum yield, and good photo-stability, they will have the potential to dramatically improve existing LSC designs. Self-absorption is the primary mechanism that limits the concentration capability of an LSC. Thus, by eliminating self-absorption, optical flux concentration can be improved and system costs can be minimized.
1.2.2.3 – Quantum Dot Nanocrystals

Quantum dot nanocrystals (QDs) are semiconducting nanoparticles that have size-tunable energy-band characteristics due to quantum confinement effects in all three spatial dimensions [23]. The size of a QD dictates the degree of confinement; decreasing the size of a quantum dot increases the energy-band spacing and band-gap accordingly. Thus, the absorption and emission spectra of QDs can be adjusted by changing their size. Since photoluminescence emission energies ($E_{PL}$) of quantum dots are dictated by their band-gap ($E_g$), which can be modified simply by changing their size, specific sizes of QDs can be matched to the spectral response of particular photovoltaic (PV) absorber materials to enhance the power conversion efficiency of LSCs.

Quantum dots fabricated from cadmium selenide (CdSe) have a strong absorption spectrum in the visible range, and have respectable fluorescence quantum yields around 0.6 [24]. Quantum dots fabricated from lead-sulfide (PbS) [25] and lead-selenide (PbSe) [26] have very broad absorption spectra and are capable of emitting photons in the infrared spectrum, as opposed to visible spectrum emission displayed by the majority of other fluorescent materials used in LSCs. A larger absorption spectrum bandwidth allows photons from a larger range of energies to be absorbed by the infrared emitting quantum dots than typical fluorescent materials that emit light in the visible spectrum. Infrared emission is also useful in LSCs because it allows for multiple LSCs to be coupled together in a tandem configuration, allowing one LSC to absorb and collect photons in the visible spectrum while another LSC underneath is capable of absorbing and collecting photons in the infrared spectrum.

The photostability and life span of QDs theoretically should be greater than most organic dyes, but it is still not as high as expected considering the inorganic semiconducting nature of quantum dots. Interestingly, some QDs exhibit the characteristic of dark-cycle recovery, whereby the defects created due to long-term, high-energy solar radiation exposure are fixed when the QDs are contained in a dark environment for a long enough period of time [27]. Due to the natural day and night cycle of earth, dark-cycle recovery is an extremely useful trait for QD LSCs since the QDs can heal overnight from the damage done by solar radiation exposure during the day.

In general, the absorption and emission spectra of QDs tends to overlap significantly. This, in addition to less-than-unity fluorescence quantum yields, causes QDs to exhibit severe self-absorption loss, which tends to be the primary drawback of using QDs as the active fluorescent material in LSCs. Minimizing self-absorption loss is one of the major challenges facing researchers in developing high quality quantum dots for use in LSCs. However, it is possible to minimize self-absorption by fabricating high quality, uniform size quantum dots with extremely narrow emission spectra, but these are more difficult and costly to manufacture than lower quality QDs with a larger size distribution. It is also possible to reduce self-absorption by taking advantage of non-radiative energy transfer mechanisms between small and large QDs.
1.2.3 – Photovoltaic Cells

The photovoltaic cells attached to the edges of an LSC should have near unity quantum efficiency at fluorescence emission wavelengths, high performance under concentrated irradiance, and low cost per unit area. The PV absorber materials used in LSC designs are typically limited to either Silicon (Si) or Gallium-Arsenide (GaAs). However, other types of PV cells such as CdTe and Organic PV cells may prove to be viable replacements for Si and GaAs due to their low cost and good spectral response at particular wavelengths that correspond well with commonly used fluorescent materials. Furthermore, PV cells can be enhanced by plasmon resonance tuned to the emission spectrum of the fluorescent material to enhance LSC power conversion efficiency [28].

1.3 – Monte Carlo Simulation

A Monte Carlo simulation is a form of numerical analysis based on the generation of random numbers and the use of applicable stochastic (probabilistic) data to form approximate solutions to both deterministic and non-deterministic problems [29], [30]. The Monte Carlo method is often used and most applicable to situations when no deterministic algorithm can be found and/or the problem variables have coupled degrees of freedom. A ray-tracing simulation is a type of mathematical model that traces out the paths of photons in a system based on the physical interaction of the photons with its surroundings. Ray-tracing takes physical phenomena into account, such as absorption, reflection, transmission, and emission, based on mathematical equations and data, such as the Beer-Lambert Law, refractive indices, absorption spectra, emission spectra, emission trajectory distribution, and many other factors.

In the case of an LSC, the mechanism of self-absorption makes it unreasonable to use simple integration and averaging to accurately calculate efficiencies. Many events that occur in an LSC are inherently probabilistic, and thus are well calculated using Monte Carlo simulation. As a result, Monte Carlo simulation is an excellent method for simulating LSC systems.

A Monte Carlo ray tracing simulation was developed using GoldSim Pro (Academic Version) to simulate and characterize a wide variety of different LSCs for this thesis. There are two principal goals of this thesis. The first and primary goal of this thesis is to develop accurate, robust, and user-friendly simulation software that can be used to analyze and optimize the photon collection capability, power conversion efficiency, and cost of conventional LSC systems. The second goal of this thesis is to use the Monte Carlo simulation software to characterize previously studied LSC materials, propose new ideas to improve efficiency and reduce cost, and perform optimization studies to assess the present and potential capability of using LSC systems to harvest solar power at reduced cost.
Chapter 2: Theory of Operation

To determine the possible paths photons may take in an LSC and the physical principles governing each interaction, the following events must be taken into consideration.

2.1 – Solar Irradiance

Solar irradiance incident on the front surface of the LSC may either reflect off of or transmit into the LSC waveguide. Figures 3a and 3b are plots of the AM1.5G solar spectrum obtained from the national renewable energy laboratory (NREL) which show spectral irradiance \( I_\lambda \) and spectral photon irradiance \( I_{\lambda p} \) vs. wavelength \( \lambda \) [31].

![Figure 3](image-url)

**Figure 3:** (a) AM1.5G solar spectral irradiance (W/m\(^2\)/nm) vs. wavelength (nm).
(b) AM1.5G solar spectral photon irradiance (#/s/m\(^2\)/nm) vs. wavelength (nm).

The peak integrated solar irradiance (photon energy flux density) incident on the surface of the earth on a perfectly sunny day under optimal conditions is about 1000 W/m\(^2\). Nearly 81% of solar irradiance and 64% of solar photon irradiance consists of photons with energies above the band-gap of silicon \( \sim \)1.1eV. However, only a fraction of this power can be converted to usable electrical power due to losses in the concentrator system and the PV cells.
2.2 – External Reflection

The majority of incident solar irradiance passes into the waveguide where it may either be absorbed by the fluorescent material or transmit through the other side, and a small fraction of incident photons are lost due to reflection off of the waveguide’s front surface. The amount of reflection is determined by the angle of incidence of light, and the index of refraction of the waveguide material.

The index of refraction \((n)\) is a material property that determines the phase velocity of light and how significantly light reflects and refracts when transmitting from one material to another at a particular angle of incidence [32]. However, refractive index is not constant; it has a slight wavelength and temperature dependence which varies for different materials. The most commonly used LSC waveguide materials are glass and polymethyl-methacrylate (PMMA; aka acrylic glass or Plexiglas), which have refractive indices of nearly 1.51 and 1.48 at 900nm, which is an optimal emission wavelength for coupling to silicon PV. Figure 4 shows a plot of refractive \((n)\) vs. wavelength for Schott BK-7 glass and acrylic glass (PMMA) at 20°C [33].

![Figure 4: a plot of refractive index \((n)\) vs. wavelength for Schott BK-7 glass at 20°C from 300nm to 1700nm and acrylic glass (PMMA) at 20°C from 400nm to 1060nm [33].](image)

The relationship between refractive index, angles of incidence and refraction, and the speed of light between two materials is defined by Snell’s Law given by equation 1,

\[
\frac{\sin \theta_i}{\sin \theta_r} = \frac{n_2}{n_1} = \frac{v_1}{v_2}, \tag{1}
\]

where \(\theta_i\) is the angle of incidence, \(\theta_r\) is the angle of refraction, \(n_1\) is the refractive index of the first medium, \(n_2\) is the refractive index of the second medium, \(v_1\) is the phase velocity of light in the first medium, and \(v_2\) is the phase velocity of light in the
second medium. A vacuum has a refractive index of 1, in which the phase velocity of light is \( c = 3 \times 10^8 \text{ m/s} \). Higher indices of refraction correspond to a slowing of light by a factor of \( 1/n \). Thus the phase velocity of light is \( c/n \) in a corresponding material with a refractive index of \( n \). For the remainder of this paper, the refractive index of the waveguide will be simply referred to as \( n \), and the refractive index of the surrounding medium will be assumed to be that of air (\( n_{air} \approx 1 \)). Since the refractive index of common waveguide materials is relatively constant over a large wavelength span, and the wavelength dependence of refractive index over the entire solar spectrum is difficult to obtain, typically it is mathematically modeled as a constant when determining LSC efficiencies to avoid unnecessary complexities in calculations.

Fresnel reflectance for perpendicular polarized light (\( R_s \)) and parallel polarized light (\( R_p \)) are determined using the equations 2 and 3 [34].

\[
R_s = \left( \frac{n_1 \cos(\theta_i) - n_2 \cos(\theta_t)}{n_1 \cos(\theta_i) + n_2 \cos(\theta_t)} \right)^2 = \left[ \frac{n_1 \cos(\theta_i) - n_2 \sqrt{1 - \left( \frac{n_1}{n_2} \sin(\theta_i) \right)^2}}{n_1 \cos(\theta_i) + n_2 \sqrt{1 - \left( \frac{n_1}{n_2} \sin(\theta_i) \right)^2}} \right]^2 \tag{2}
\]

\[
R_p = \left( \frac{n_1 \cos(\theta_t) - n_2 \cos(\theta_i)}{n_1 \cos(\theta_t) + n_2 \cos(\theta_i)} \right)^2 = \left[ \frac{n_1 \sqrt{1 - \left( \frac{n_1}{n_2} \sin(\theta_i) \right)^2} - n_2 \cos(\theta_i)}{n_1 \sqrt{1 - \left( \frac{n_1}{n_2} \sin(\theta_i) \right)^2} + n_2 \cos(\theta_i)} \right]^2 \tag{3}
\]

Sunlight can be assumed to be non-polarized. The reflectance (\( R \)), or probability of non-polarized photon reflection at the interface of two media, is determined by averaging \( R_s \) and \( R_p \) as shown in equation 4.

\[
R = \frac{R_s + R_p}{2} \tag{4}
\]

If \( \theta_i \approx 0^\circ \), \( n_1 \approx 1 \), and \( n_2 = n \), the non-polarized reflectance can be simplified to equation 5.

\[
R = \left( \frac{n - 1}{n + 1} \right)^2 \tag{5}
\]

In addition to reflectance, the transmittance (\( T \)), or probability of photon transmission at the interface of two media, is defined simply as the converse probability of reflectance as shown in equation 6.

\[
T = 1 - R \tag{6}
\]

Fresnel reflection typically only accounts for \( \sim 4\% \) loss for common waveguide materials at small angles of incidence. However, as the angle of incidence increases beyond \( 60^\circ \), reflectance becomes much more significant. Anti-reflective coatings can
help to reduce the amount of reflection at the air/glass interface, but with added cost. Figure 5 shows a plot of reflectance \( R \), perpendicular polarization reflectance \( R_s \), and parallel polarization reflectance \( R_p \) vs. angle of incidence \( \theta_i \) for photons incident on an air/glass interface of an LSC waveguide with \( n = 1.5 \).

![Air - to - Glass Reflectance](image)

**Figure 5:** Reflectance \( R \), perpendicular polarization reflectance \( R_s \), and parallel polarization reflectance \( R_p \) vs. angle of incidence \( \theta_i \) for photons transmitting from air to a glass LSC waveguide with \( n = 1.5 \).

The flux \( \Gamma \), or quantity flowing through a surface per unit time, can be calculated using equation 7,

\[
\Gamma = \iiint_{S} \Phi \cdot dS
\]  

(7)

where \( \Phi \) is the flux density, or quantity flowing through a surface per unit area per unit time and \( dS \) is a differential area element pointing normal to the surface. Photon flux \( (\Gamma_p) \), photon energy flux \( (\Gamma'_p) \), photon flux density \( (\Phi_p) \), and photon energy flux density \( (\Phi'_p) \) (a.k.a. irradiance) are likewise defined. Since solar photons incident on a small section of the Earth can be assumed to be traveling in plane waves (in other words, the solar photons are traveling approximately parallel to each other), and the front LSC face is assumed to be planar, \( \Gamma \) is more simply defined as,

\[
\Gamma = |\Phi \cdot A_{LSC}| = \Phi A_{LSC} \cos(\theta_i)
\]

(8)

where \( \cos(\theta_i) \) represents the fraction of photon flux incident on the front surface of the LSC relative to the maximum attainable incident photon flux. The product of \( \cos(\theta_i) \)
and the transmittance into the waveguide will be defined as the peak-flux-transmittance ($T_{\text{flux}}$) and is calculated using equation 9.

$$T_{\text{flux}} = \cos(\theta_i) \ (1 - R)$$  \hfill (9)

Figure 6 shows a plot of peak-flux-transmittance ($T_{\text{flux}}$) vs. angle of incidence ($\theta_i$) for photons incident on an air/waveguide interface of an LSC waveguide with $n = 1.5$.

![Air-to-Waveguide Peak-Flux-Transmittance](image)

**Figure 6:** a plot of peak-flux-transmittance ($T_{\text{flux}}$) vs. angle of incidence ($\theta_i$) for photons at an air/waveguide interface of an LSC waveguide with $n = 1.5$.

Although LSCs are touted as excellent absorbers of diffuse and off-angle solar radiation, it is still important to keep in mind that reflection and flux loss from indirect placement of the LSC relative to the incident angle of solar radiation will yield significant losses. However, as long as the angle of incidence in direct sunlight is less than $33^\circ$, more than 80% of solar irradiance will transmit into the LSC waveguide. At near perfect incidence angles, nearly 96% of solar irradiance will transmit into the LSC and be capable of subsequent absorption, emission, entrapment, collection, and photo-conversion.
2.3 – Absorption

Fluorescent particles absorb a fraction of the incident photons depending on the absorption spectrum, concentration, and thickness of the fluorescent material. The absorption and transmission of photons at a given wavelength is characterized using the Beer-Lambert law [35],

\[ I = I_0 e^{-\alpha L}, \]  

where \( I \) is the intensity of photons after traversing an optical path length of \( L \), \( I_0 \) is the intensity of the incident photons, \( \alpha \) is the material’s absorption coefficient and \( L \) is the optical path length through the material. The absorption coefficient is further defined as,

\[ \alpha = \varepsilon c_x, \]

where \( \varepsilon \) is the naperian molar absorptivity of the fluorescent material and \( c_x \) is the concentration of the fluorescent material. Molar absorptivity is an intrinsic, wavelength-dependent material property, whereas concentration can be varied by increasing or decreasing the amount of absorber material per unit volume.

Figure 7 is a plot of the absorption spectra (fractional absorption vs. wavelength) of PbSe QDs dispersed in tetrachloroethylene in a 5mm thick cuvette with solution concentrations of 0.35, 1.1, 5.3, and 39.6μM.

![Figure 7: A plot of absorption spectra (fractional absorption vs. wavelength) of PbSe QDs for solution concentrations 0.35, 1.1, 5.3, and 39.6μM in a 5mm thick cuvette.](image-url)
An absorption spectrum is a plot of the intensity or probability of photon absorption as a function of wavelength, where the intensity of absorption at each wavelength may either be defined by the fractional absorbance \((A)\), the absorption coefficient at a particular concentration \((\alpha)\), or intrinsically by the absorptivity \((\varepsilon)\). The absorption spectrum of the fluorescent material used in an LSC should be broad to absorb as much solar irradiance as possible, and have little to no overlap with its own emission spectrum.

The fractional absorption of photons at a particular wavelength \((A)\) is defined by,

\[
A = 1 - e^{-\alpha L}.
\]

The molar absorptivity for a given fluorescent material at each wavelength can be found from a material’s absorption spectrum (fractional absorption vs. wavelength) using equation 13 if the concentration and optical path length are known.

\[
\varepsilon = -\frac{\ln(1 - A)}{c_x L}.
\]

Knowing the molar absorptivity spectrum of a fluorescent material used in a given LSC system is extremely useful for mathematical modeling since it allows the absorption coefficient and fractional absorption at any solution concentration and optical path length to be calculated. By increasing the concentration and thickness of the fluorescent material in an LSC, the fractional absorption at each wavelength can be enhanced due to the increasing number of fluorescent particles that photons must interact with before passing through the LSC. However, increasing the solution concentration also increases the probability of self-absorption due to absorption/emission spectrum overlap. Also, increasing the LSC thickness reduces the geometric concentration factor of the LSC, which reduces the maximum photon flux concentration capability of the system.

Absorption is one of the most critical components of an LSC, but concentration and absorber thickness must be carefully balanced with other parameters to ensure optimal photon collection and photon flux concentration are obtained. The fraction of incident photons and the fraction of incident power absorbed by the fluorescent material in an LSC are known as the photon absorption efficiency \((\eta_{abs})\) and power absorption efficiency \((\eta'_{abs})\) respectively and are defined by equations 14 and 15,

\[
\eta_{abs} = \frac{\text{Photons Absorbed}}{\text{Incident Photons}} = \frac{\int I_{p\lambda} T_{\text{flux}} A d\lambda}{\int I_{p\lambda} d\lambda},
\]

\[
\eta'_{abs} = \frac{\text{Power Absorbed}}{\text{Incident Power}} = \frac{\int I_{p\lambda} T_{\text{flux}} A d\lambda}{\int I_{p\lambda} d\lambda},
\]

where \(I_{p\lambda}\) is the spectral photon irradiance, \(I_{\lambda}\) is the spectral irradiance, \(T_{\text{flux}}\) is the peak-flux transmittance, and \(A\) is the fractional absorbance of the fluorescent material.
2.4 – Emission

Photon absorption is one of the many mechanisms in nature that is capable of promoting electrons to higher energy states. If photon absorption excites an electron and the excited electron emits a new photon by relaxing from a higher energy state to a lower energy state, it is known as fluorescence or photoluminescence (PL). More generally, if electron-excitation by any mechanism produces a photon when the electron relaxes from a higher energy state to a lower energy, it is known as radiative relaxation (RR). If a photon is not emitted after absorption, the electron energy transition from a higher energy state to a lower energy state contributes to generating vibrations (heat) or exciting other electrons in the material, and is known generally as non-radiative relaxation (NRR). The probability of radiative relaxation occurring in a fluorescent material per photon absorbed is defined by its fluorescence quantum yield ($\eta_{QY}$), also known simply as quantum yield.

\[
\eta_{QY} = \frac{\text{# emitted photons}}{\text{# absorbed photons}}
\]

Fluorescence quantum yield is one of the most important parameters for high efficiency LSCs since it determines not only the emission probability of absorbed solar photons, but also the emission probability of self-absorbed photons as well. Optimally, $\eta_{QY}$ should be as close to unity as possible. Organic fluorescent materials often display $\eta_{QY} > 0.9$ [21], but inorganic fluorescent materials such as semi-conducting quantum dots usually display $\eta_{QY} < 0.7$ except in rare cases such as PbSe QDs which have reported $\eta_{QY}$ values as high as 0.89 [36], but there is some debate regarding the validity of these high $\eta_{QY}$ measurements [37].

The emission or PL spectrum of a fluorescent material, as shown in figure 8 for PbSe QDs, is the range of wavelengths that are emitted by a fluorescent material and the relative intensity of emission at each wavelength.

![Figure 8: Absorption (fractional absorbance vs. wavelength) and emission (normalized photoluminescence intensity vs. wavelength) spectra of PbSe QDs with a concentration of 5.3µM. The emission peak is normalized to the first-absorption peak for ease of comparison. The wavelength difference between the PL emission peak (1515nm) and the first absorption peak (1465nm) corresponds to a 50nm stokes shift.](image.png)
The emission spectrum of a fluorescent material used in an LSC must optimally have no overlap with its respective absorption spectrum, must be relatively narrow, and must couple well with available photovoltaic absorber materials. If the photon emission energies are lower in energy than the band-gap of the photovoltaic absorber material, they cannot be absorbed and harvested. If the photon emission energies are too much higher than the band-gap of the photovoltaic absorber material, much of the energy will be lost to thermalization. The Stokes shift of a fluorescent material is defined as the shift in wavelength between the peak emission intensity and first (lowest energy) absorption peak. Stokes efficiency in an LSC is defined as the average fraction of absorbed photon energy remaining after emission occurs, and can be approximated using the following equation,

$$\eta_{Stokes} = \left( \frac{\hbar c}{\lambda_{PL}} \right) \frac{\int_{\lambda} I_{\lambda} T_{\lambda} A \, d\lambda}{\int_{\lambda} I_{\lambda} T_{\lambda} A \, d\lambda},$$

where \(\hbar\) is Planck’s constant \((6.63\times10^{-34} \text{ J-s})\), \(c\) is the speed of light in a vacuum \((3.0\times10^{8} \text{ m/s})\), and \(\lambda_{PL}\) is the average collected PL emission wavelength. The first quantity represents the average collected photon emission energy and the second quantity represents the average absorbed solar photon energy.

Once a fluorescent particle emits a photon, there is a possibility for six distinct events to occur, as illustrated for a single fluorescence emission center in figure 9.

![Illustrated cross-section of an LSC with six possible emission paths](image)

**Figure 9:** Illustrated cross-section of an LSC with six possible emission paths: collection, entrapment due to TIR, escape-cone loss, partial reflection, self-absorption, and host-absorption.

First, there is a possibility that a photon will be emitted in a direction resulting in direct collection at one of the LSC edges without any prior internal reflection. Second, there is a possibility that the photon will be emitted at an angle such that the angle of incidence is greater than the critical angle, resulting in total internal reflection (TIR); this mechanism is known as entrapment. Third, there is a small probability that a photon will be emitted at an angle inside the escape-cone region where the angle of incidence is less than the critical angle, but still be reflected due to Fresnel reflection; this mechanism is
known as partial reflection. Fourth, regardless of which direction the photon travels after emission, the emitted photon may be reabsorbed by another fluorescent particle inside the LSC where it has a possibility of being re-emitted by radiative relaxation or quenched by non-radiative relaxation; this mechanism is known as self-absorption. Fifth, there is a probability that the photon will be emitted at an angle such that it is lost by transmission through the front or back face of the LSC; this loss mechanism is known as escape-cone loss due to the imaginary cone that can be drawn to illustrate the region of loss around the emission center. Sixth, rarely, it’s possible for the solvent or the host matrix to absorb and quench fluorescence emission (and solar photons); this mechanism is known as host-absorption but will be ignored in this thesis due to its low probability of occurrence. These events will be discussed in detail in sections 2.5, 2.6, and 2.7.

2.5 – Internal Reflection

The primary operating mechanism of photoluminescence entrapment in an LSC is total-internal-reflection. Total-internal-reflection is caused by the interaction of light at the interface of two media such that light is transmitting from a medium with a larger index of refraction to a medium with a smaller index of refraction and the angle of incidence is greater than the critical angle \( \theta_c \) defined by Snell’s Law. These conditions result in near-perfect reflection \( (R \approx 1) \) of light at the interface.

The critical angle \( \theta_c \) is the threshold angle of incidence at which light is refracted parallel and coplanar to the interface plane, and is found using equation 18 derived by solving Snell’s law for \( \theta_i \) if \( \theta_t = 90^\circ \). When \( \theta_i = \theta_c, \theta_t = 90^\circ \). If \( \theta_i < \theta_c \), some of the photons reflect while others transmit and consequently refract. If \( \theta_i > \theta_c \), photons will undergo total internal reflection.

\[
\theta_c = \sin^{-1}(1/n)
\]  

(18)

Though PL in many fluorescent particles tends to have a preferred direction, the random orientation of particles in an LSC system allows for the assumption that global PL emission is isotropic; i.e. photons have an equal probability of being emitted in any direction. If isotropic PL emission is assumed, the probability of TIR entrapment for a single emission event, also known as trapping efficiency \( \eta_{\text{trap}} \), is determined by the refractive index of the waveguide material and can be calculated using equation 19 [10],

\[
\eta_{\text{trap}} = \frac{\sqrt{n^2 - 1}}{n} = \cos(\theta_c),
\]  

(19)

where \( n \) is the index of refraction of the waveguide and \( \theta_c \) is the critical angle of reflection. If isotropic emission is assumed and partial reflection is ignored, the probability of escape-cone loss for a single emission event is equal to the converse probability of entrapment \( (1 - \eta_{\text{trap}}) \). A conventional LSC waveguide with \( n \) of 1.5 will yield \( \eta_{\text{trap}} \) of 74.5%. Though \( \eta_{\text{trap}} \) is proportional to \( n \), no suitable waveguide materials
have been discovered with \( n \) significantly greater than 1.5. Theoretical waveguides with \( n \) of 2 and 3 would yield \( \eta_{\text{trap}} \) of 86.6% and 94.3% respectively.

Escape-cone loss is slightly mitigated due to partial reflection, or reflection occurring when either a transmitted solar photon or emitted photon with an emission angle \( \theta < \theta_c \) is reflected at the waveguide/air interface in an LSC. Figure 10 shows a plot of reflectance (\( R \)), perpendicular polarization reflectance (\( R_s \)), and parallel polarization reflectance (\( R_p \)) vs. angle of incidence (\( \theta_i \)) for photons at a waveguide/air interface of an LSC made of glass with \( n = 1.5 \).

![Glass - to - Air Reflectance](image)

**Figure 10:** A plot of reflectance (\( R \)), perpendicular polarization reflectance (\( R_s \)), and parallel polarization reflectance (\( R_p \)) vs. angle of incidence (\( \theta_i \)) for photons at a waveguide/air interface of an LSC waveguide made of glass with \( n = 1.5 \). Though individual fluorescent particles may have a preferred emission direction and polarization, large quantities of randomly oriented particles allows for the assumption that emission is non-polarized. The asymptotic behavior near 41.81° and near-perfect reflection at \( \theta_i > 41.81^\circ \) is due to total internal reflection.

Although partial reflection improves the overall LSC absorption efficiency and trapping efficiency, the contribution of this mechanism to LSC efficiency is extremely small due to the fact that light that undergoes partial reflection has a high probability of escape-cone loss on the opposite side of the LSC unless the photon is self-absorbed and subsequently reemitted at an angle greater than the critical angle. Escape-cone loss may also be mitigated by photons absorbed so closely to the edge of an LSC that PL emission with \( \theta_i < \theta_c \) is directly collected by the PV cell before the photon reaches the front or back surface of the LSC; i.e. direct collection at \( \theta_i < \theta_c \). However, collection due to this mechanism is relatively inconsequential because partial reflection may also occur at the LSC edges as well, thus hindering PL transmission from the LSC to the PV cell absorber material.
Typical PV absorber materials such as crystalline silicon (c-Si), polycrystalline silicon (pc-Si), amorphous silicon (a-Si:H), gallium arsenide (GaAs), and germanium (Ge), have complicated wavelength-dependent indices of refraction typically ranging between 2 and 6 [33]. Therefore, the intrinsic Fresnel reflectance of these materials is typically higher than 30% in air and 10% in glass for $\theta_i = 0^\circ$. However, since fluorescent materials used in LSCs have a narrow PL emission wavelength range, anti-reflective coatings can be tailored to the refractive index of the waveguide and PV absorber material at PL emission wavelengths. Since anti-reflective coatings tend to work best at a specific wavelength range and angle of incidence, the reflectance of PL emission can be minimized to nearly zero for $\theta_i = 0^\circ$ and greatly minimized for other angles of incidence. Additional losses may occur due to imperfect LSC-PV contact, but these losses can be assumed to be negligible for a properly fabricated system.

2.6 – Self-Absorption

Self-absorption arises when a photon previously emitted by a fluorescent particle is reabsorbed by another fluorescent particle; if a self-absorbed photon is subsequently lost to either non-radiative recombination or escape-cone transmission, it is defined as self-absorption (or reabsorption) loss [11]. Self-absorption loss is currently one of the largest problems inhibiting high efficiency LSCs. The amount of self-absorption in a fluorescent material is dependent on the degree of overlap between its absorption and emission spectra, which is sometimes characterized by the Stokes shift. Since self-absorption is essentially the only mechanism that can produce optical losses after entrapment, a quantity called self-absorption efficiency ($\eta_{SA}$) can be calculated using equation 20,

$$\eta_{SA} = \frac{\eta_{opt}}{\eta_{abs} \eta_{QY} \eta_{trap}} \cong (\eta_{QY} \eta_{trap})^{N_{SA}},$$

where $N_{SA}$ is the average number of self-absorptions a photon undergoes after entrapment, and $\eta_{opt}$ is the optical efficiency of the LSC. Since $N_{SA}$ is difficult to calculate without the aid of a computer due to the complex relationships between PL wavelength, PL emission direction, self-absorption probability, and optical path length to an edge, it is often easier to first calculate self-absorption efficiency after optical efficiency has already been determined.

Non-radiative relaxation loss and escape-cone transmission are separable into two categories depending on whether the photon was lost during the initial absorption/emission event or after self-absorption occurs. The probability of re-emission is defined by $\eta_{QY}$ of the fluorescent material used in the LSC. In general, materials with low $\eta_{QY}$ suffer from much more significant self-absorption losses relative to the amount of trapped photons in the system than materials with high $\eta_{QY}$. The combination of absorption/emission band overlap and fluorescence quantum yield of the fluorescent material will determine the relative losses associated with self-absorption in the LSC.
2.7 – Efficiency

Collection occurs if an emitted photon traveling through an LSC transmits through one of the LSC edges. Subsequent absorption and energy conversion in the photovoltaic cell allows the LSC to produce useful electrical work. The efficiency of an LSC system is characterized by four principal quantities: optical efficiency ($\eta_{opt}$), integrated external quantum efficiency ($\eta_{EQE}$), LSC power conversion efficiency ($\eta_{PCE}$), and power conversion flux gain ($F_{PCE}$), which will be further discussed in the following subsections. Monte-Carlo simulations can be used to easily determine LSC efficiencies due to the probabilistic nature of reflection, transmission, absorption, emission, entrapment, self-absorption, and photo-conversion.

2.7.1 – Optical Efficiency

The optical efficiency of an LSC is defined in several ways depending on the reference, but can be generally defined as the fraction incident photons or fraction of incident power collected by the concentrator. Optical efficiency ($\eta_{opt}$) and optical-power efficiency ($\eta'_{opt}$) are characterized and theoretically determined using equations 21 and 22 respectively,

$$\eta_{opt} = \frac{\text{# collected photons}}{\text{# incident photons}} = \eta_{abs} \eta_{QY} \eta_{trap} \eta_{SA}$$

$$\eta'_{opt} = \frac{\text{collected power}}{\text{incident power}} = \eta_{abs} \eta_{Stokes} \eta_{QY} \eta_{trap} \eta_{SA}$$,

which are only a function of the concentrator itself and have no relation to the PV cells attached to the edges. Optical efficiency is useful for comparing the light collection efficiency of different fluorescent materials with similar emission wavelengths [38]. Since PV cells have a limited detection range, a third type of optical efficiency which will be referred to as electronic optical efficiency ($\eta^e_{opt}$), defined by equation 23, is often used during experimental LSC characterization when it is necessary to estimate the fraction of collected photons relative to the absorption range of the attached PV cells [39].

$$\eta^e_{opt} = \frac{\text{# detected photons}}{\text{# detectable incident photons}} = \frac{I_{LSC} A_{PV}}{I_{PV} A_{LSC}} = \frac{1}{G} \frac{I_{LSC}}{I_{PV}}$$,

where $I_{LSC}$ is the short circuit current produced by the PV cells when attached to the LSC, $I_{PV}$ is the short circuit current produced by the PV cells when not attached to the LSC, $A_{LSC}$ is the front surface area of the LSC, and $A_{PV}$ is the area of the PV cells attached to the LSC edges. It is also useful to think $\eta^e_{opt}$ as a measure of the photocurrent generated by the LSC-PV system at short-circuit relative to the photocurrent that would be generated by a PV cell in direct sunlight with an absorption area equal to $A_{LSC}$.
2.7.2 – Quantum Efficiency

Photovoltaic cells have a limited photon absorption and conversion range due to their band-gap energy ($E_g$) and wavelength-dependent quantum efficiency (QE). Therefore, not all of the collected photons will be converted to photocurrent in the PV cell. The EQE (IQE) of a PV cell is defined as the fraction of incident (absorbed) photons that are converted to photocurrent in the PV cell at short-circuit operating conditions. Solar cell EQE measurements take external reflection into account while IQE does not. Therefore, IQE will always be greater than or equal to EQE. Figure 11 shows a plot of EQE and IQE vs. wavelength for a mono-crystalline silicon solar cell [40].

**Figure 11**: A plot of external quantum efficiency (EQE) and internal quantum efficiency (IQE) vs. wavelength for a mono-crystalline silicon solar cell, adapted from [40]. Quantum efficiency typically goes to zero at photon energies less than the band-gap unless significant localized-state-to-band energy transitions take place.

Quantum efficiency typically drops to zero at wavelengths beyond the cutoff wavelength ($\lambda_c$) defined by equation 24,

$$\lambda_c = \frac{h c}{E_g},$$  \hspace{1cm} (24)

where $E_g$ is the band-gap energy of the semiconducting PV absorber material. In an LSC, it is essential for fluorescent material emission wavelengths to correspond with high PV QE to optimize LSC power conversion efficiency. Due to the relatively narrow emission spectra of typical fluorescent materials, anti-reflection coatings and optical gels tailored to the waveguide-PV interface allow emitted photons to transmit from the LSC to the PV cell with low loss.
The integrated LSC external quantum efficiency ($\eta_{EQE}$) is defined by equation 25

$$\eta_{EQE} = \frac{\# \text{extracted electrons}}{\# \text{incident photons}} = \frac{1}{q_e} \left( \frac{I_{LSC}}{\Phi A_{LSC}} \right) = \eta_{opt} \text{EQE}(\lambda_{PL}),$$  \hspace{1cm} (25)

where $q_e$ is the elementary charge of an electron of $1.602 \times 10^{-19}$ C, $I_{LSC}$ is the short-circuit current generated by the PV cells attached to the LSC, and $\text{EQE}(\lambda_{PL})$ is the average EQE of the attached solar cells at the collected emission wavelengths.

### 2.7.3 – Power Conversion Efficiency

The LSC power conversion efficiency ($\eta_{PCE}$) is defined as,

$$\eta_{PCE} = \frac{P_{out}}{P_{in}},$$  \hspace{1cm} (26)

where $P_{out}$ is the output power of the PV cells attached to the LSC and $P_{in}$ is the radiant power incident on the front surface of the LSC. Experimentally, $\eta_{PCE}$ is very easy to determine since $P_{out}$ can be measured directly. Theoretically, $\eta_{PCE}$ can be approximated by the product of $\eta_{opt}$ and the monochromatic power conversion efficiency of the attached PV cells at the collected emission wavelengths ($\eta_{PV}(\lambda_{PL})$). Otherwise, $\eta_{PCE}$ can also be approximated using the solar cell diode equations if $\text{EQE}(\lambda_{PL})$, the dark saturation current ($I_0$) of the PV cell, the fill factor of the PV cell, and $\eta_{opt}$ of the LSC are known.

To maximize $P_{out}$ and $\eta_{PCE}$, the solar cells attached to the LSC should be operating at their maximum power points. The maximum power point of a PV cell can be represented as,

$$P_{MP} = V_{MP} I_{MP} = V_{OC} I_{SC} FF,$$  \hspace{1cm} (27)

where $V_{MP}$ is the voltage produced at the maximum power point, $I_{MP}$ is the current generated at the maximum power point, $V_{OC}$ is the open-circuit voltage, $I_{SC}$ is the short-circuit current, and FF is the fill factor. Fill factor is the fraction of power produced at the maximum power point relative to unobtainable power product of $V_{OC}$ and $I_{SC}$ as shown equation 28.

$$FF = \frac{V_{MP} I_{MP}}{V_{OC} I_{SC}}$$  \hspace{1cm} (28)

The maximum power point is found by varying the voltage bias applied to a PV cell under illumination until the product of voltage and current is maximized. Figure 12 shows a plot of an I-V curve for a solar cell, adapted from [41].

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Figure 12: A current vs. voltage (IV) curve for a solar cell, adapted from [41]. Fill factor is the ratio between the area encompassed by the shaded rectangle and the product of $V_{OC}$ and $I_{SC}$.

The power conversion efficiency of an LSC will almost always be less than that of using attached PV cells in direct sunlight due to transmission, escape-cone, and non-radiative recombination loss, but flux gain is ultimately the more important parameter governing the performance of an LSC system.

2.7.4 – Flux Gain

Before flux gain can be determined, the LSC geometric gain ($G$) must first be calculated using equation 29 [42].

$$G = \frac{A_{LSC}}{A_{PV}}$$  \hspace{1cm} (29)

The geometric gain is a measure of the maximum possible photon flux concentration of an LSC assuming all other factors are perfect and lossless. A balanced geometric gain is essential for the proper operation of an LSC. If $G$ is too low, light will not be concentrated very strongly, but LSC efficiencies will be high. Unfortunately, many researchers use this fact to their advantage when reporting high-efficiency LSC devices. As $A_{LSC}$ diminishes, the prevalence of self-absorption reduces; as $A_{PV}$ increases, the fraction of incident photons absorbed by the LSC increases. If $G$ is too high, self-absorption loss and/or reduced solar photon absorption will reduce LSC efficiencies. Consequently, geometric gain must be balanced to obtain adequate light concentration without sacrificing efficiency. It has been cited in research that a geometric gain on the order of 10 is suitable for achieving a balance between efficiency and flux gain [42], but it will ultimately depend on the fluorescent material and the requirements for a particular application.
Flux gain may be defined generally as the photonic flux gain \( F_{opt} \) or photonic energy flux gain \( F'_{opt} \) of an LSC as shown in the following equations,

\[
F_{opt} = G \eta_{opt} \tag{30}
\]

\[
F'_{opt} = G \eta'_{opt} \tag{31}
\]

However, LSC flux gain \( F_{PCE} \) is traditionally defined as the gain in power output per unit PV cell area from using a concentrator system relative to using the attached PV cells in unconcentrated light. In this sense, flux gain measures the effective power conversion concentration factor of an LSC. A more suitable name for LSC flux gain would be power conversion gain since it is not necessarily directly proportional to either the photon or photon-energy flux gain. Nevertheless, LSC flux gain \( F_{PCE} \) is calculated using equation 32 [43],

\[
F_{PCE} = G \frac{\eta_{PCE}}{\eta_{PV}} \tag{32}
\]

where \( \eta_{PCE} \) is the power conversion efficiency of the LSC with attached PV cells, and \( \eta_{PV} \) is the power conversion efficiency of the PV cells without attaching them to the LSC. For an LSC to be practical, \( F_{PCE} \) must be greater than 1, otherwise the inherent purpose of the LSC is lost and the concentrator system is actually functioning effectively as a luminescent solar diffuser instead of a solar concentrator. Consequently, achieving \( F_{PCE} \) greater than 1 is absolutely required for an effective LSC device. The fundamental goal when designing a luminescent solar concentrator device is to maximize the flux gain without sacrificing power conversion efficiency by optimizing design parameters and minimizing loss.

2.8 – Cost

The cost per watt peak of an LSC is the most important factor governing its commercial viability. The ability for solar energy conversion to compete with other forms of energy production is dependent upon the ability of scientists and engineers to create and install solar conversion systems capable of producing power for less than $1/W_p [44]. Currently, Silicon based PV modules (typically with \( \eta_{PV} \) between 12% and 16%) can be purchased for around $1.50/W_p [45], and CdTe based photovoltaic modules (with \( \eta_{PV} \) typically between 10% and 12%) can be purchased for less than $1.00/W_p [46], but these costs do not include installation costs. For LSCs to be commercially successful, they must be able to substantially concentrate light to reduce the cost per watt of the PV cells attached to the LSC relative to the cost per watt of the same PV cells in AM1.5 sunlight. Additionally, the waveguide, fluorescent material, assembly, and other miscellaneous costs associated with the production process must not exceed the PV cell cost savings associated with light concentration.
The installation cost of implementing photovoltaic modules into a building or home often constitutes a large portion of the overall costs associated solar power generation. As the price of solar cell manufacturing goes down, installation costs become large in comparison. Since LSC systems can double as windows and solar cells, the use of LSCs in window installations can partially alleviate installation costs and help to promote BIPV. However, the addition of a back-surface reflector would render an LSC useless in such an application. Even if LSCs aren’t used in place of windows, they may still be successful if their cost reduction capability offsets their reduced power conversion efficiency.

The dollar per watt peak production cost of an LSC ($/$\text{W}_p)_{LSC}$ can be estimated using a simplified cost model [43] based on equation 33,

\[
\frac{$}{\text{W}_p}_{LSC} = \frac{\$_{LSC}}{P_{in} \eta_{PCE}}, \tag{33}
\]

where $\$_{LSC}$ is the cost of the entire LSC system with the attached PV cells, and $P_{in}$ is the input solar power. Since the cost of PV cells is often cited in units of $/$\text{W}_p, and $1/F_{PCE}$ represents the cost per watt reduction factor of the PV cells due to light concentration, the cost-per-watt of the LSC system can be rewritten as,

\[
\frac{$}{\text{W}_p}_{LSC} = \frac{\$_{\text{conc}}}{P_{in} \eta_{PCE}} + \frac{1}{F_{PCE}} \left( \frac{$}{\text{W}_p}_{PV} \right), \tag{34}
\]

where ($/$\text{W}_p)$_{PV}$ is the cost-per-watt of the attached PV cells in peak sunlight (1000W/m$^2$), and $\$_{\text{conc}}$ is the cost of the solar concentrator without the attached PV cells. For greater specificity, $\$_{\text{conc}}$ can be separated into the following components: waveguide material cost ($\$_{wg}$), fluorescent material cost ($\$_{fm}$), optional back-surface reflector cost ($\$_{BSR}$), assembly cost ($\$_{asm}$), and miscellaneous cost ($\$_{misc}$). However, assembly costs are difficult to determine because they are dependent upon the manufacturing processes of the LSC rather than the cost of raw materials.

Waveguide cost is typically inversely proportional to the quantity of material ordered and the scale of mass production, but typically on the order of 1¢/cm$^3$. Two common waveguides used in LSCs, Glass and PMMA, cost approximately 0.7¢/cm$^3$ and 0.48¢/cm$^3$ respectively [40]. Due to the variability in material costs with production scale, these values serve only as order of magnitude estimates based on results reported by literature. Fluorescent material costs are also dependent on the scale of mass production, which makes organic dyes much more cost effective than quantum dots at the present time. Quantum dots typically sell for anywhere between $100/g and well over $1000/g [47], whereas organic dyes are several orders of magnitude less expensive and typically cost around $20/g [40]. However, this cost disparity is likely related to different scales of production rather than the intrinsic value of the materials used in the production process.
2.9 – LSC Design Modifications

Although $\eta_{\text{trap}}$ is fixed for a given waveguide material and $\eta_{\text{abs}}$, $\eta_{\text{QY}}$, $\eta_{\text{Stokes}}$, and $\eta_{\text{sA}}$ are relatively fixed for a given concentration of fluorescent material in a simple LSC system, it is possible to reduce losses and improve efficiencies with several LSC design modifications.

2.9.1 – Back-Surface Reflector (BSR)

The most simple and least expensive method of simultaneously improving $\eta_{\text{abs}}$ and $\eta_{\text{trap}}$ is to use a mirror or white scattering layer at the back surface of the LSC. Using either a mirror or a white scattering layer increases the reflection probability of both transmitted solar photons and emitted photons that transmit through the back face of the LSC. Photons, which would have otherwise been lost, have a chance to be reflected and absorbed or collected at an edge of the LSC. Figure 13 shows a schematic of an LSC with a BSR.

![Back-Surface Reflector](image)

**Figure 13:** Schematic cross-section of an LSC system utilizing a back-surface reflector (BSR) to reflect solar photons and PL emitted photons at the back-surface to either be reabsorbed by the fluorescent material or collected at an edge.

Research has shown between a 37% and 50% optical efficiency improvement from using a white scattering layer at the back surface of the LSC, but silver mirrors typically only work half as well [48]. White scattering layers tend to perform better than silver mirrors because diffuse reflection changes the direction of incident/reflected photons such that $\theta_i \neq \theta_r$, thereby increasing the average optical path-length available for photons to be absorbed. Additionally, scattered solar photons have a chance to reflect at an angle such that they are collected by the PV cell without undergoing absorption at all. However, the efficiency gain obtained from using either a white scattering layer or a specular mirror is entirely dependent upon the optical properties of the fluorescent material and the other design parameters of the LSC.
2.9.2 – Thin-Film LSC

Most LSC systems utilize fluorescent materials doped within a waveguide host-matrix to absorb and emit photons. However, it is also possible to separate the waveguide and the fluorescent material by placing a dense thin-film of fluorescent material on the front or back surface of the waveguide as shown in figure 14.

![Thin-Film Fluorescent Material](image)

**Figure 14:** Schematic cross-section of a thin-film LSC system utilizing a film of fluorescent material placed on the front surface of the LSC as opposed to filling the bulk of the waveguide with fluorescent material. A portion of the emission directed downward will become trapped with no self-absorption loss in the waveguide until next time the photon reaches the top surface.

It is often necessary to use extremely high concentrations of the fluorescent material to achieve adequate absorption when a thin film is used. Unfortunately, it is common to see a reduction of $\eta_{QY}$ at high fluorescent material concentrations due to aggregation and quenching effects [38]. On the other hand, high fluorescent material concentration can be beneficial due to the possibility of Förster resonance energy transfer between fluorescent particles [12] as will be discussed in section 2.9.4.

Recent research done by Giebink et al. has shown that it is possible to pattern the thin-film across the LSC such that wave-properties of light force emission modes to be directed into the LSC at particular angles [20]. By optimizing the thin-film structure of the fluorescent material to control the surfaces at which light interacts, the light trapping efficiency of an LSC can be improved beyond the limit of $\eta_{trap}$ defined by equation 19. If this design principle can be further exploited, it has the potential to tremendously improve the limits of $\eta_{opt}$, $\eta_{PCE}$, and especially $F_{PCE}$.
2.9.3 – Tandem LSC

Another method of improving device efficiency whilst reducing escape cone losses is to use multiple stacks of LSCs, known as a tandem LSC system, as shown in figure 15. Using tandem LSCs allows light to be separated into any number of individual LSCs, each with a different fluorescent material that has a different absorption/emission spectrum. Thus, tandem LSC configurations have the ability to greatly improve the efficiency of LSC systems by spectrally separating the solar spectrum [43].

![Illustrated cross-section of a tandem LSC system utilizing a stack of three LSCs with different fluorescent materials. Solar and escape-cone transmission from LSCs higher in the stack may be absorbed by LSCs lower in the stack. Consequently, escape cone loss is minimized, solar absorption is maximized, and LSC efficiency is improved.](image)

**Figure 15:** Illustrated cross-section of a tandem LSC system utilizing a stack of three LSCs with different fluorescent materials. Solar and escape-cone transmission from LSCs higher in the stack may be absorbed by LSCs lower in the stack. Consequently, escape cone loss is minimized, solar absorption is maximized, and LSC efficiency is improved.

Generally, fluorescent materials only absorb light with energies greater than their emission peaks. Thus, by placing an LSC that absorbs/emits light at the smallest wavelengths (highest energies) on top and placing an LSC that absorbs/emits light at the largest wavelengths (lowest energies) on the bottom, the light will separate into individual spectra for each LSC to effectively absorb, concentrate, and couple to appropriate PV cells. Additionally, if photons are lost from the escape cone of one LSC, it is possible for the photon to be reabsorbed and utilized by another LSC in the stack.

Though there is much useful energy to be harvested from the infrared spectrum, most fluorescent materials do not efficiently absorb and emit light in the infrared range. However, PbSe QDs are a potential candidate for the fluorescent material in an infrared harvesting LSC layer due to their high $\eta_{QY}$ relative to infrared emitting organic dyes and absorption spectrum spanning into the infrared spectrum, beyond the cutoff wavelength of silicon. The potential use of PbSe QDs as a fluorescent material in an infrared harvesting LSC layer was first proposed and studied in this research, and is discussed in Chapter 5.
2.9.4 – Förster Resonance Energy Transfer (FRET)

Förster resonance energy transfer (FRET), also known as fluorescence resonance energy transfer, is an energy transfer mechanism between two types of fluorescent particles, often labeled as “donors” and “acceptors”, whereby incident photon energy absorbed by a donor may non-radiatively transfer to an acceptor, which may subsequently result in acceptor PL emission [49]. Figure 2 shows an illustrated schematic of FRET occurring between donor and acceptor particles.

![Illustrated schematic of FRET](image)

**Figure 16:** Illustrated schematic representation of Förster resonance energy transfer occurring between an arbitrary donor and acceptor. A donor may either fluoresce directly after absorption or transfer the absorbed energy non-radiatively to an acceptor depending on the FRET efficiency.

Förster resonance energy transfer was discovered in the 1940’s by the German chemist Theodor Förster. It is often used in biological sensing and sometimes referred to as a “spectroscopic ruler” due to its extreme sensitivity to inter-particle spacing distance [50]. As it is understood, FRET interaction is based on dipole-dipole resonance coupling between fluorescent particles. Its prevalence is dependent upon the relative orientations of donor and acceptor dipole moments, degree of overlap between donor emission and acceptor absorption spectrum spectra, the spacing distance between donor and acceptor, the fluorescence quantum yield of the donor, and the refractive index of the surrounding medium.

Though it is important for the emission spectrum of the donor to overlap with the absorption spectrum of the acceptor to ensure high FRET efficiency, energy absorbed by the donor is transferred completely non-radiatively, as opposed to radiative energy transfer that occurs during self-absorption. This makes intuitive sense from a quantum mechanical standpoint because there must be an available energy level in the acceptor to receive the amount of energy provided by the donor. Furthermore, from a quantum-electrodynamical standpoint, FRET interaction occurs due virtual photon interaction between donors and acceptors, which also explains why the donor/acceptor emission/absorption spectra must overlap [51].
It is important to note, there is always a possibility for FRET to occur between two supposed donors or two supposed acceptors if the inter-particle spacing distance is small enough and all other necessary FRET conditions are met; if this scenario occurs, it will functionally be as if FRET did not occur at all. To increase the probability of successful FRET interaction and reduce the prevalence of self-absorption among homogeneously dispersed, close packed fluorescent particles, donor concentration should typically higher than acceptor concentration (D/A ratio > 1) to ensure that donors are absorbing a greater portion of incident photons than acceptors and to ensure that the prevalence of acceptor self-absorption is reduced. However, if the donor/acceptor concentration ratio becomes too large, the dominance of donors over acceptors will reduce the probability of successful and functional FRET due to both lack of available acceptors and competing intra-donor FRET [49]. Functional FRET may occur within a single type of QD material when large quantum dots and small quantum dots are in close proximity. If the conditions for FRET are met, energy absorbed by the smaller quantum dots (donors) will non-radiatively transfer to the larger quantum dots (acceptors), leading to an overall larger absorption spectrum and a stronger emission peak at the longer PL wavelength and lower energy associated with the larger quantum dots.

The FRET mechanism effectively separates the net absorption and emission spectra to that of the donor and acceptor respectively. As a result, the wavelength separation distance between the absorption and emission peaks, otherwise known as the Stokes shift, can be greatly enhanced if FRET occurs among properly selected donors and acceptors. Fluorescent materials with large Stokes shifts are highly desired for LSC applications because it reduces the prevalence of self-absorption, a problem that has plagued LSC development since its incarnation in the late 1970’s. Theoretically, utilizing FRET coupled fluorescent particles in an LSC system should yield improved flux concentration, optical efficiency, and power conversion efficiency compared to using donors or acceptors exclusively due to enhanced absorption and reduced self-absorption loss. However, due to the close proximity required between fluorescent particles on the order of nanometers for FRET to work, LSCs utilizing FRET must be fabricated as thin-film LSCs.
Chapter 3: LSC Monte Carlo Ray-tracing Simulation

3.1 – LSC Simulation Algorithm

The algorithm used to create the Monte Carlo simulation discussed in this paper is shown in flow chart form in figure 17.

Figure 17: LSC Monte Carlo ray-tracing simulation algorithm flow chart
Each time a realization of the model is run, only one randomly generated photon is accounted for. For this single photon, the goal is to detect whether it will be collected at one of the edge faces of the LSC and subsequently whether or not it will be converted to photocurrent in the PV cell. If the photon does not reach an edge of the LSC, the simulation also determines if and when the photon is lost due to reflection, transmission, or non-radiative recombination.

3.2 – Assumptions

A large number of assumptions were made to model an LSC with the Monte Carlo method using GoldSim Pro software. Even though the AM1.5G solar spectrum, which includes both direct and off-angle radiation, is used to generate light, all light impinging on the system is assumed to have normal incidence relative to the front surface of the LSC. The refractive index of the fluorescent particles embedded inside the host matrix is assumed to be the same as the host matrix. The refractive index of the waveguide is assumed to be constant and independent of photon wavelength. Scattering and wave interference effects are ignored. Host absorption in the waveguide is ignored.

The luminescent particles in solution are assumed to be dispersed homogenously throughout the LSC system; thus, the absorption spectrum is constant throughout the LSC system. Host matrix modification of the absorption and emission spectrum of the fluorescent material is ignored. The fluorescence quantum yield of the fluorescent material is assumed to be constant, regardless of concentration and incident photon energy. Applicable to all fluorescent materials but with specific reference to quantum dots, Auger multiplication, also known as multiple exciton generation (MEG), is ignored regardless of incident photon energy. At high dye concentrations and otherwise, photoluminescence quenching effects and non-radiative energy transfer mechanisms are ignored. Photoluminescence redshift is modeled by only allowing emission wavelengths to be greater than or equal to all previous emission wavelengths.

Reflection at the waveguide edges and LSC/PV coupling losses are completely ignored; i.e. the PV cells attached to the edges of the LSC are assumed to be perfectly coupled with an appropriate anti-reflective coating or optical gel. Superposition is assumed to be valid for all simulated solar cells. Fill factor is assumed to be constant with reference to the performance of the solar cell under AM1.5 irradiance. Solar cells attached to the LSC edges are assumed to be connected in parallel. Shunt resistance is ignored. The ideality factor of the solar cells is assumed to be unity. The temperature of the solar cells attached to the edges of the LSC is assumed to be constant at 300K. If a tandem LSC is used, coupling between solar cells in the top and bottom LSC is ignored; total tandem LSC efficiency is recorded as the efficiency sum of the two LSC systems. If a tandem LSC is used, light reflection and propagation at the interfaces within the air gap of the two LSCs is ignored. If a BSR is used, light reflection at the LSC/air interface and propagation within the air gap is also ignored. The total cost of an LSC only accounts for the material costs of the waveguide, fluorescent material, solar cells, and back surface reflector; manufacturing and miscellaneous costs such as material preparation and energy consumption are ignored.
3.3 – Photon Generation

The first step in the LSC algorithm is to generate an incident photon ($\lambda_i$) from a probability density function (PDF) that models the solar spectrum. A PDF is a function that shows the probability of occurrence for a randomly selected value in a specified domain. The integral of a PDF from the lower to the upper limit of its domain is equal to one. However, GoldSim Pro only allows a custom PDF to be generated from a cumulative distribution function (CDF). A CDF is a continuous function that shows the probability that a randomly generated value from a PDF will be less than or equal to a specified value in the domain, and is calculated by integrating its respective PDF. Data provided by NREL that models the AM1.5G spectral photon irradiance as a function of wavelength was converted to a CDF by numerical integration and subsequent normalization, and uploaded to GoldSim Pro to represent the solar spectrum in this model. Figure 18 shows the PDF and CDF of the AM1.5 spectrum.

![Figure 18](image)

Figure 18: The AM 1.5G spectral photon irradiance cumulative distribution function (top) and corresponding probability density function (bottom) in GoldSim Pro.
3.4 – External Reflection

Once a random photon wavelength is generated from the solar spectrum PDF, the probability of reflection at the front surface of the LSC must be calculated from the Fresnel reflection equations defined by equations 2 - 5. Since the angle of incidence is assumed to be normal to the front face of the LSC, sunlight is assumed to be non-polarized, the temperature of the LSC is assumed to be constant, and the index of refraction of the LSC is assumed to be independent of photon wavelength, the probability of a photon reflecting off of the top surface of the LSC is determined solely by the user-defined, constant index of refraction of the waveguide material. Thus, the probability of reflection is calculated using the non-polarized Fresnel reflectance equation defined by equation 5, \( R = [(n - 1)/(n + 1)]^2 \). Since most waveguides used in LSCs have an index of refraction near 1.5, the probability of reflection is nearly 4% for each photon generated in the Monte Carlo simulation. If a photon is reflected, it is accounted for as a loss in GoldSim and a new realization begins. If a photon is not reflected, the program continues to determine whether or not the solar photon is absorbed in the LSC or not.

3.5 – Absorption

Once a photon enters into the LSC, the probability of absorption must be calculated. To determine whether absorption takes place or not, the absorption path length \( L_{abs} \) and optical path length \( L_{opt} \) must be determined and compared. The absorption path length is the distance the generated photon with wavelength \( \lambda_i \) must travel within the LSC system before it is absorbed. The optical path length is the distance a photon travels through the LSC before it is transmitted through the front or back surface. If \( L_{opt} < L_{abs} \), the photon will transmit through the LSC before it is absorbed. If \( L_{opt} > L_{abs} \), the photon will be absorbed when it has traveled a total distance of \( L_{abs} \).

The absorption path length is based on the concentration of the fluorescent material \( c_x \) and the naperian molar absorptivity spectrum \( \varepsilon(\lambda) \) of the fluorescent material at the generated photon wavelength. The concentration of the fluorescent material is defined by the user. The absorptivity spectrum must be defined by the user for a range of wavelengths. If a photon is generated with a wavelength outside the range of \( \varepsilon(\lambda) \), \( L_{abs} \) is calculated using either endpoint of \( \varepsilon(\lambda) \) (depending on whether the generated photon wavelength is less than the smallest defined wavelength or greater than the largest defined wavelength). If the user desires no absorption to take place outside the bounds of \( \varepsilon(\lambda) \), the user must bound the spectrum with some finite \( \varepsilon \) approaching zero at the endpoints of \( \lambda \). The fractional absorbance, \( A = 1 - e^{-\alpha z} \), where \( \alpha = \varepsilon c_x \), is a cumulative distribution function modeling the probability that a photon will be absorbed at or before distance \( z \). The associated probability density function is determined by taking the spatial derivative of the fractional absorbance as shown in equation 35,

\[
\frac{dA}{dx} = \alpha e^{-\alpha z}
\] (35)
Thus, the rate of absorption per unit length is a probability density function governed by a negative exponential distribution with a mean of $\alpha = \varepsilon (\lambda_i) c_x$. This function can be input into a stochastic element in GoldSim Pro to randomly generate $L_{abs}$ for the generated photon.

The optical path length of a photon in an LSC is dependent upon the thickness of the LSC ($t_{LSC}$) and how many times the photon reflects inside the LSC ($N_R^{abs}$) due to either Fresnel reflection or BSR reflection. If internal reflection is completely ignored, the optical path length is simply equal to $t_{LSC}$. The required number of times a photon must reflect before it is absorbed is determined by the absorption path length and the thickness of the LSC and can be calculated using equation 36.

$$N_R^{abs} = \text{Trunc} \left[ \frac{L_{abs}}{t_{LSC}} \right]$$ (36)

If the photon is approaching a surface without an additional reflection layer, the probability of reflection is calculated using the Fresnel reflectance equation defined by equation 4. For photons with normal angles of incidence and waveguides with an index of refraction near 1.5, the probability of internal reflectance is nearly 4%. If the photon is approaching the back surface and an additional BSR layer is used, the reflectance, i.e. the probability of reflection, is defined by the user. A loop is used to determine whether or not the photon is reflected or transmitted each time it interacts with the top or bottom interface, and whether or not the photon was absorbed or not on each pass. Each time the photon is reflected, $L_{opt}$ increases by $t_{LSC}$. If $L_{opt} > L_{abs}$, the photon is absorbed, counted toward $n_{abs}$, and the x-y coordinate of the fluorescent particle $(x_p, y_p)$, as shown in figure 19, is determined randomly from uniform probability distributions spanning the width ($W_{LSC}$) and length ($L_{LSC}$) of the LSC respectively. The z-coordinate of the fluorescent particle $(z_p)$, shown in figure 19, is determined using the following expressions.

$$\text{If } N_R^{abs} = \text{even, } z_p = t_{LSC} \left[ 1 - \left( \frac{L_{abs}}{t_{LSC}} - N_R^{abs} \right) \right]$$ (37)

$$\text{If } N_R^{abs} = \text{odd, } z_p = t_{LSC} \left( \frac{L_{abs}}{t_{LSC}} - N_R^{abs} \right)$$
Figure 19: Schematic 3D view of an LSC: The x,y,z coordinate of the fluorescent particle that absorbed the photon is referenced as \((x_p, y_p, z_p)\), and the width, length, and thickness of the LSC are referenced as \(W_{LSC}\), \(L_{LSC}\), and \(t_{LSC}\) respectively.

If the photon is transmitted and a tandem LSC is not used, it is counted as transmission loss. If the photon transmits through the back surface of the LSC and a tandem LSC is used, the generated photon will transmit into the tandem LSC where the absorption process reiterates for the material parameters of the tandem LSC. If it is not necessary to know which surface the photon transmits through, a loop is actually unnecessary and computationally wasteful; in this case, the probability that the photon will be reflected inside the LSC enough times to be absorbed \((P_r^{abs})\) can be calculated using the following expressions.

\[
\text{If } N_R^{abs} = \text{even}, \quad P_r^{abs} = R_{Back}^{N_R^{abs} / 2} R_{Front}^{N_R^{abs} / 2} \\
\text{If } N_R^{abs} = \text{odd}, \quad P_r^{abs} = R_{Back}^{(N_R^{abs} + 1) / 2} R_{Front}^{(N_R^{abs} - 1) / 2}
\]

(38)

3.6 – Emission

Once a photon is absorbed (or reabsorbed), the probability of photoluminescence emission is simply defined by the fluorescence quantum yield \((\eta_{QY})\) of the fluorescent material. Emission is determined by comparing \(\eta_{QY}\) to a random number generated between 0 and 1. If the random number is greater than \(\eta_{QY}\), the photon is not emitted and the assumed to be lost due to non-radiative relaxation (NRR). If the random number is less than \(\eta_{QY}\) a photon is emitted and the wavelength of the emitted photon \((\lambda_{PL})\) is determined from a probability density function modeling the emission spectrum of the fluorescent material.
3.7 – Trajectory

If emission occurs, the next step is to determine the trajectory of the emitted photon. Since emission is assumed to be isotropic, the probability density function that models $\phi$ is defined by a uniform distribution of $1/2\pi$ between 0 and $2\pi$, and the probability density function that models $\theta$ is defined by $\sin(\theta)/2$ between 0 and $\pi$ [52] as shown in figure 20.

![Figure 20: Illustration of PL emission trajectory angles in spherical coordinates and plots of the corresponding probability density functions for isotropic emission.](image)

A formal way of deriving these distribution functions is by assuming the probability density of photons emitted per solid-angle ($\Omega$) is constant and normalized to $1/4\pi$ in accordance to the total surface area of a unit sphere. Since a differential solid angle can be converted to spherical coordinates by, $d\Omega = \sin(\theta) d\theta d\phi$, the probability density functions between a solid-angle and spherical coordinates can be related by the equation, $\rho(\Omega) = \sin(\theta) P(\theta)P(\phi)$. Thus, $P(\theta)P(\phi) = \sin(\theta)/4\pi$. By integrating the product of $P(\theta)P(\phi)$ over $\phi$ to obtain $P(\theta)$, and vice versa, the probability density functions modeling isotropic emission in spherical coordinates can be derived.

Although it may seem counter-intuitive that both probability density functions are not uniform to obtain isotropic directionality, insight can be obtained by imagining $\phi$ sweeping from 0 to $2\pi$ with constant $\theta$. Near the poles, at $\theta \sim 0$ and $\theta \sim \pi$, the arc-length swept by the ray and $\phi$ on an imaginary unit sphere is very small. On the other hand, near the equator at $\theta \sim \pi/2$, the arc-length swept by the ray and $\phi$ on an imaginary unit sphere is very large. Since the average number of photons emitted per circumferential arc must be constant, $\theta$ must have a higher probability of incidence near the equator than the poles, which results in a sin distribution for isotropy.
Since the x, y, and z starting coordinates and trajectory of the photon are known, the resultant path that the photon is required to traverse to reach an edge is fixed unless self-absorption or escape-cone transmission occur. Before the 3D path length to the LSC edge (\(L_{xyz}\)) can be determined, the program must calculate where the photon trajectory intersects one of the four edges of the LSC. To simplify this calculation, the photon trajectory is projected onto the x-y plane shown in figure 21, and calculated using one of the following expressions.

1) If \(2\pi - \tan^{-1} \left( \frac{y_p}{W_{LSC} - x_p} \right) \leq \phi < \left[ \tan^{-1} \left( \frac{L_{LSC} - y_p}{W_{LSC} - x_p} \right) \right] \), \[ L_{xy} = \left| \frac{W_{LSC} - x_p}{\cos(\phi)} \right| \]

2) If \(\tan^{-1} \left( \frac{L_{LSC} - y_p}{W_{LSC} - x_p} \right) \leq \phi < \left[ \pi - \tan^{-1} \left( \frac{L_{LSC} - y_p}{x_p} \right) \right] \), \[ L_{xy} = \left| \frac{L_{LSC} - y_p}{\sin(\phi)} \right| \]

3) If \(\pi - \tan^{-1} \left( \frac{L_{LSC} - y_p}{x_p} \right) \leq \phi < \left[ \frac{3\pi}{2} - \tan^{-1} \left( \frac{x_p}{y_p} \right) \right] \), \[ L_{xy} = \left| \frac{x_p}{\cos(\phi)} \right| \]

4) If \(\frac{3\pi}{2} - \tan^{-1} \left( \frac{x_p}{y_p} \right) \leq \phi < \left[ 2\pi - \tan^{-1} \left( \frac{y_p}{W_{LSC} - x_p} \right) \right] \), \[ L_{xy} = \left| \frac{y_p}{\sin(\phi)} \right| \]

Figure 21: Aerial view schematic of an LSC with the photon trajectory and path length to the edge projected onto the x-y plane. The trigonometric relationships between the trajectory and \(L_{xy}\) depend on which edge the photon trajectory intersects. Edges 1, 2, 3, and 4 correspond to the right, top, left, and bottom edges of the LSC as referenced from the schematic [53].
Trigonometric relationships between $x$, $y$, $W_{LSC}$, and $L_{LSC}$ are used to determine where the photon trajectory intersects with an edge of the LSC and the 2D path length to the LSC edge in the x-y plane ($L_{xy}$) [53]. After $L_{xy}$ is calculated, $L_{xyz}$ can be determined by projecting the reflected path onto a straight line that is collinear to the original path length before reflection occurs [53], as shown in figure 22. This calculation can only be made by assuming that every reflection at the top and bottom surfaces satisfies the condition $\theta_i = \theta_r$. If this condition is not satisfied, as is the case for white scattering layers which produce a Lambertian distribution for $\theta_R$, a new trajectory must be calculated each time the photon reflects at an interface, which is not accounted for in this simulation.

![Figure 22: Section view of a trapped photon in an LSC. Since $\theta_i = \theta_r$, by projecting the path of the photon onto a single line, the total 3D path length to the edge can be calculated using trigonometry. It is interesting to note that the z-coordinate of the fluorescent particle is inconsequential. The 3D path length to the edge can be determined entirely from $x_p, y_p, \phi$, and $\theta$.](image)

\[ L_{xyz} = \frac{L_{xy}}{\sin \theta'} \]  

(40)

Once $L_{xyz}$ is calculated, it needs to be compared to the self-absorption path length ($L_{SA}$). The self-absorption path length is determined using the negative exponential distribution PDF, $\alpha e^{-\alpha x}$, where $\alpha = \pi (\lambda PL) c_x$ [53]. Assuming the photon does not transmit through the LSC during any of the reflection events: if $L_{xyz} < L_{SA}$, $L'_{xyz} = L_{xyz}$ and the photon will reach an edge of the LSC before it is self-absorbed, else if $L_{SA} < L_{xyz}$, $L'_{xyz} = L_{SA}$ and the photon will be self-absorbed after traveling a distance of $L_{SA}$. However, it is not yet known whether or not the photon will actually traverse the total 3D path length of $L'_{xyz}$ because the probability of reflection has not yet been taken into account.
Assuming the photon does traverse $L'_{\text{xyz}}$ with the trajectory $\phi$ and $\theta$, the new $x$, $y$, and $z$ coordinates of the photon, $x'_p, y'_p, z'_p$ are calculated using the following expressions.

\begin{align*}
x'_p &= x_p + L'_{\text{xyz}} \sin \theta \cos \phi, \quad (41) \\
y'_p &= y_p + L'_{\text{xyz}} \sin \theta \sin \phi, \quad (42)
\end{align*}

If $\theta < \pi/2$ and $N_R$ is even,
\[ z'_p = t_{\text{LSC}} \left[ \text{MOD} \left( \frac{z_p + L'_{\text{xyz}} \cos(\theta)}{t_{\text{LSC}}}, N_R \right) \right], \]
If $\theta < \pi/2$ and $N_R$ is odd,
\[ z'_p = t_{\text{LSC}} \left[ 1 - \text{MOD} \left( \frac{z_p + L'_{\text{xyz}} \cos(\theta)}{t_{\text{LSC}}}, N_R \right) \right]. \]
If $\theta > \pi/2$ and $N_R$ is even,
\[ z'_p = t_{\text{LSC}} \left[ 1 - \text{MOD} \left( 1 - \frac{z_p + L'_{\text{xyz}} \cos(\theta)}{t_{\text{LSC}}}, N_R \right) \right], \quad (43) \\
If $\theta > \pi/2$ and $N_R$ is odd,
\[ z'_p = t_{\text{LSC}} \left[ \text{MOD} \left( 1 - \frac{z_p + L'_{\text{xyz}} \cos(\theta)}{t_{\text{LSC}}}, N_R \right) \right]. \\
If $\theta = \pi/2$,
\[ z'_p = z_p \]

Where $N_R$ is the number of reflections necessary for the photon to traverse $L'_{\text{xyz}}$, assuming $\theta_i = \theta_R$, which is calculated with the following expressions.

\begin{align*}
\text{If } \theta < \pi/2, & \quad N_R = \text{TRUNC} \left( \frac{z_p + L'_{\text{xyz}} \cos(\theta)}{t_{\text{LSC}}} \right), \\
\text{If } \theta > \pi/2, & \quad N_R = \text{TRUNC} \left( 1 - \frac{z_p + L'_{\text{xyz}} \cos(\theta)}{t_{\text{LSC}}} \right), \quad (44) \\
\text{If } \theta = \pi/2, & \quad N_R = 0,
\end{align*}

MOD is the modulus function which reports the remainder of the first argument divided by the second argument and TRUNC is the truncate function which reports the integer value of the argument by removing all of the digits after the decimal place. The conditions necessary to select the appropriate $z'_p$ and $N_R$ functions can be reduced, albeit with additional complication, by utilizing the Heaviside step function, $H[\theta]$, which is defined as 1 when the argument is positive and 0 when the argument is negative.

\begin{align*}
\text{If } \theta \neq \pi/2, & \quad z'_p = t_{\text{LSC}} \left[ \Psi + (-1)^w \text{MOD} \left( \Omega + (-1)^\alpha \frac{z_p + L'_{\text{xyz}} \cos(\theta)}{t_{\text{LSC}}}, N_R \right) \right], \\
N_R & = \text{TRUNC} \left( \Omega + (-1)^\alpha \frac{z_p + L'_{\text{xyz}} \cos(\theta)}{t_{\text{LSC}}} \right), \quad (45)
\end{align*}

where,
\[ \Psi = \text{MOD}[\Omega + \text{MOD}(N_R, 2), 2]. \]
\[ \Omega = H \left( \theta - \frac{\pi}{2} \right) \]
3.8 – Entrapment

Photon entrapment is determined by calculating the probability that the emitted photon will reflect enough times within the LSC to traverse the path length $L'_{xyz}$ ($P_R$). Assuming the fluorescent particle emits light with random polarization, this probability is determined by the exponentiation of the non-polarized Fresnel reflection coefficient ($R$) by $N_R$ as shown in equation 46.

$$P_R = \left\{ \frac{1}{2} \left[ \frac{n \cos(\theta) - \sqrt{1 - (n \sin(\theta))^2}}{n \cos(\theta) + \sqrt{1 - (n \sin(\theta))^2}} \right]^2 + \frac{n \sqrt{1 - (n \sin(\theta))^2}}{n \sqrt{1 - (n \sin(\theta))^2} + \cos(\theta)} \right\}^{N_R} , \quad (46)$$

As $\theta \to \theta_c$, $R$ approaches unity as seen previously in figure 10. If $\theta > \theta_c$, total internal reflection (TIR) occurs; in this case, $P_R$ is always equal to 1.

In the case that a BSR is used and TIR does not occur, the probability of reflection off of the back surface ($R_{\text{Back}}$) may be different than the probability of reflection off of the front surface ($R_{\text{Front}}$). In this case, the program accounts for the fact that the reflectance is different at the front and back interface as shown in the following equations.

$$\text{If } N_R = \text{even}, \quad P_R = R_{\text{Back}}^{\frac{N_R}{2}} R_{\text{Front}}^{\frac{N_R}{2}}$$

$$\text{If } N_R = \text{odd}, \quad P_R = R_{\text{Back}}^{\frac{1}{2} \left( \frac{N_R}{2} + \frac{\theta - \pi/2}{|\theta - \pi/2|} \right)} R_{\text{Front}}^{\frac{1}{2} \left( N_R - \frac{\theta - \pi/2}{|\theta - \pi/2|} \right)}$$

After $P_R$ is calculated, a random number between 0 and 1 is generated and compared to $P_R$. If the random number is greater than $P_R$, the photon is lost due to escape-cone loss at some number of reflections between 1 and $N_R$. If a tandem LSC is used and the emitted photon is lost through the back-surface of the LSC, the photon passes into the tandem LSC where the processes determining absorption, emission, trajectory, and outcome will repeat for the material properties of the tandem LSC.

If the random number is less than $P_R$ and $L'_{xyz}$ represents the self-absorption path length, the photon will be self-absorbed at $x'_p, y'_p, z'_p$, and the program will begin a new emission event using $x'_p, y'_p, z'_p$ as the new, initial position of the fluorescent particle $x_p, y_p, z_p$. In which case, the simulation will repeat the processes determining emission, trajectory, and outcome until the photon is either collected or lost. If the random number is less than $P_R$ and $L'_{xyz}$ represents the collection path length to an edge, the photon will be collected at an edge of the LSC and counted toward $\eta_{opt}$. 

40
3.9 – Photocurrent Generation

If the photon is collected at an edge of the LSC, it may contribute to generating photocurrent in the attached solar cell. To determine whether or not the emitted, collected photon will generate current at short-circuit operating conditions, the external quantum efficiency at the collected emission wavelength (EQE(λPL)) is compared to a random number generated between 0 and 1. The EQE(λ) spectrum of the solar cell is defined by the user and must be bounded such that EQE → 0 at the endpoints if photocurrent generation is undesired outside of the bounds of the spectrum. If the random number between 0 and 1 is greater than EQE(λPL), the photon will either not be absorbed by the solar cell, or the generated free electron hole pair will recombine; in either case, the photon contributes to ηopt, but does not contribute to ηEQE. If the random number is less than EQE(λPL), the photon will generate photocurrent in the attached solar cell at short-circuit and contribute to ηEQE.

3.10 – Post-Processing

The processes described above in sections 3.5 – 3.10 will repeat for the number of realizations defined by the user. At the end of the simulation, results from all realizations are compiled to determine the fraction of incident photons and energy absorbed (ηabs), collected (ηopt), converted to short-circuit photocurrent (ηEQE), lost to direct transmission (T) lost to NRR before self-absorption (NRRl), lost to NRR after self-absorption (NRRSA), lost to escape-cone transmission before self-absorption (ECl), and lost to escape-cone transmission after self-absorption (ECSA). Additionally, the average number of times a photon is self-absorbed (NSA), average energy of generated photons (Eph), average energy of collected photons (EPL), optical flux gain (Fopt), and other similar parameters are stored.

It is important to note that time is not involved in the simulation process. Therefore, the user must specify the incident photon flux density (Φin) and photon energy flux density (Φin') of the incident spectrum to determine the number of photons and radiant energy incident on the LSC per unit time. With these quantities, the amount of power incident on the LSC (Pin) and the number of photons incident on the LSC per unit time (Γin) can be determined using equations 48 and 49.

\[ P_{in} = \Phi_{in}' A_{LSC} \] (48)

\[ \Gamma_{in} = \Phi_{in} A_{LSC} \] (49)

With the results of the Monte Carlo simulation in hand, the electrical output of the solar cells attached to the LSC and the estimated cost of the LSC can be determined.
3.10.1 – PV Cell Output

As discussed in section 3.7.3 the power conversion efficiency of an LSC is determined simply by the ratio of output power and input power. Since \( P_{in} \) was defined in the previous section as the product of \( \Phi_{in} \) and \( A_{LSC} \), and \( P_{out} = P_{MP} \), can be represented as the product of \( I_{SC} \), \( V_{OC} \), and \( FF \) as defined in section 3.7.3, \( \eta_{PCE} \) is calculated using equation 50.

\[
\eta_{PCE} = \frac{P_{MP}}{P_{in}} = \frac{I_{SC} \cdot V_{OC} \cdot FF}{\Phi_{in} \cdot A_{LSC}}
\]  
(50)

To estimate \( I_{SC}, V_{OC}, \) and \( FF \) for the illumination conditions present at the edges of the LSC, the solar cell diode equations are implemented [54]. The following calculations assume that superposition is valid (i.e. \( J = J_{SC} - J_{DK} \)) and shunt resistance is ignored. The dark saturation current \( (I_0) \) of a PV cell is proportional to the recombination present in the dark. Since \( J_{SC} \approx J_{DK} \) at \( V_{OC} \) and \( I_0 \) is independent of the photons absorbed in the PV cell, \( I_0 \) can be calculated using the solar cell diode equation for any reference \( I_{SC} \) and \( V_{OC} \) values specified for the attached PV cells as shown in equation 51.

\[
I_0 = \frac{I_{SC}^{0} \cdot \eta_{EQE}}{e^{\eta_{EQE}} - 1}
\]  
(51)

where \( I_{SC}^{0} \) is the reference short-circuit current, \( V_{OC}^{0} \) is the reference open-circuit voltage, \( q_e \) is the elementary charge of an electron, and \( \eta_{EQE} \) is known as the ideality factor of the diode or PV cell which is typically assumed to be 1. The short-circuit current of the LSC-PV system under illumination is calculated using equation 52,

\[
I_{SC} = q_e (\Gamma_{in} \cdot \eta_{EQE})
\]  
(52)

The product of \( \Gamma \) and \( \eta_{EQE} \) represents the total number of photons converted to photocurrent per second at short-circuit conditions. Using the calculated values of \( I_0 \) and \( I_{SC} \), the resulting open-circuit voltage can be estimated by employing the solar cell diode equation once again as shown in equation 53.

\[
V_{OC} = \frac{n \cdot k \cdot T}{q_e} \ln \left( \frac{I_{SC}}{I_0} + 1 \right)
\]  
(53)

Since the fill factor of a PV cell tends to remain relatively consistent over a range of \( I_{SC} \) [40], it is assumed to be constant, and the maximum power point of the LSC can be calculated from the product of \( V_{OC}, I_{SC}, \) and \( FF \). Additionally, the power conversion efficiency of the PV cells at the collected emission wavelengths, or photoluminescence conversion efficiency (\( \eta_{PLCE} \)), can be estimated with equation 54.

\[
\eta_{PLCE} = \frac{\eta_{PCE}}{\eta_{opt}}
\]  
(54)
3.10.2 – LSC Cost

The cost of an LSC is arguably the most important parameter to optimize in an LSC design because it will determine whether or not an LSC is commercially successful. Unfortunately, it is also the most difficult parameter to determine due to the complexities and uncertainties of the manufacturing process, fluctuating cost of materials, and price scaling. In this simulation, the cost of an LSC, as previously discussed in section 2.8, is calculated using equation 55 which only accounts for the cost of the waveguide, fluorescent material, attached solar cells, and back surface reflector if applicable. Assembly and miscellaneous costs are dependent on the facilities and methods used to fabricate the LSC, and are not estimated in this research.

\[
\left( \frac{\$}{W_{LSC}} \right) = \frac{\$_{wg} + \$_{fm} + \$_{BSR}}{p_{in} \eta_{PCE}} + \frac{1}{F_{PCE}} \left( \frac{\$}{W_{pv}} \right)
\]  

(55)

This calculation only provides a rough estimate of the total material costs involved with an LSC. To obtain the total cost, one needs to factor in not only the assembly and other miscellaneous costs involved with the production process, but also shipping and installation cost. Regardless, by assuming the same manufacturing process will be involved with all different LSC configurations, the cost figure provided by the simulation will reveal the relative costs of using different materials, but not necessarily an accurate figure for the total system cost.

The cost-per-watt of the PV cells is determined from literature. The cost of the waveguide, fluorescent material, and back-surface reflector are determined using equations 56, 57, and 58.

\[
\$_{wg} = (A_{LSC} \times t_{LSC}) \times (\$/cm^3)_{WG},
\]  

(56)

\[
\$_{fm} = c_x (A_{LSC} \times t_x) \times (\$/g)_{FM},
\]  

(57)

\[
\$_{BSR} = (A_{LSC}) \times (\$/m^2)_{BSR},
\]  

(58)

Where \(A_{LSC}\) is the front surface area of the LSC, \(t_{LSC}\) is the thickness of the LSC, \(t_x\) is the thickness of the LSC that contains fluorescent material (which is typically equal to \(t_{LSC}\) unless a thin-film or liquid solution based LSC is used), \(c_x\) is the concentration of the fluorescent material, and \((\$/cm^3)_{WG}\), \((\$/g)_{FM}\), and \((\$/m^2)_{BSR}\) are the cost per unit of the waveguide, fluorescent material, and back-surface reflector respectively. Reducing the thickness of an LSC not only reduces the waveguide and fluorescent material cost, it also increases the geometric gain which allows for higher flux gain. Although reducing the front area will reduce the cost of all three components, it also reduces the geometric gain, which limits the maximum flux gain and overall effectiveness of the LSC.
3.11 – User-Interface

The ability to implement a robust user-interface (UI), perform multi-variable sensitivity analyses, and perform multi-variable optimization studies are some of the key features that distinguish GoldSim Pro. The dashboard element in GoldSim Pro allows modelers to create input boxes, check boxes, list boxes, combo boxes, sliders, pictures, etc and couple them to elements within the model to create a front-end for his or her program. The UI created for the LSC Monte Carlo ray-tracing simulation of this thesis is shown in figure 23.

![Dashboard user-interface of the LSC Monte Carlo ray-tracing simulation.](image)

The UI enables a user to specify which materials they would like to use to model and adjust simulation parameters to change how the model behaves. Material properties are uploaded from Excel spreadsheets with reference data when the simulation begins. After running the simulation, the results can be viewed in the dashboard window below the UI shown in figure 24, in the model viewer, or in an automatically generated Excel spreadsheet.

![Dashboard results window of the LSC Monte Carlo ray-tracing simulation.](image)
3.12 – Sensitivity Analysis and Optimization

Sensitivity analyses are used to determine the relative impact one or more variables have on an output of a model. Typically, the modifiable design variables include width, length, thickness and fluorescent material concentration for a given set of LSC materials (waveguide, fluorescent material, and PV cells). It is also useful to see how outputs change with respect to fixed material parameters such as quantum yield, index of refraction, and Stokes-shift to gain insight to the effects that different material properties have on the output of the model. Moreover, sensitivity analyses can be used to tune and optimize the number of realizations simulated in a Monte Carlo model to minimize time and CPU load while maintaining a high degree of accuracy. Figure 25 shows the sensitivity analysis interface of GoldSim Pro with some of the modifiable design parameters of an LSC.

![Sensitivity Analysis Interface](Image)

Figure 25: Sensitivity analysis window of GoldSim Pro. Plots can be used to see the individual sensitivity analysis of a single variable. A Tornado chart visualizes data based on a greatest to lowest sensitivity ordered horizontal bar-chart. Result data displays individual variable sensitivity information in table form. An X-Y function chart shows a normalized plot of the dependent variable as a function of each independent variable.

Optimization studies are performed to achieve the maximum or minimum possible result for a dependent variable in a model. Optimization studies are extremely useful for LSC simulations because they can optimize all of the modifiable system properties until the highest efficiency or flux gain is achieved or the lowest cost is achieved. Without a computer program, it would be extremely difficult, if not impossible to properly optimize an LSC to achieve the lowest cost-per-watt configuration since the cost-per-watt of an LSC is dependent upon optimizing the width, length, thickness, and fluorescent material concentration to maximize the appropriate balance between power...
conversion efficiency and flux gain and while at the same time minimizing the volume of the waveguide, mass of the fluorescent material, and required area of solar cells to reduce material costs. Furthermore, GoldSim Pro allows a user to select conditions the model must satisfy within the optimization. For example, minimizing LSC cost-per-watt is extremely important, but if the efficiency of an LSC is too low, it won’t be able to generate a useful amount of electrical power. Thus, a user can optimize the simulation for lowest \(($/W)_{LSC}\), and set a limiting condition such that \(\eta_{PCE}\) must be greater than a specified value, for example 5%. Conversely, a user can optimize the simulation for highest \(\eta_{PCE}\), and set a limiting condition such that \(($/W)_{LSC}\) must be less than a specified value, for example $1.00/W. Figure 26 shows the optimization study interface of GoldSim pro, along with a realistic case study for optimizing power conversion efficiency.

**Figure 26:** Optimization window of GoldSim Pro.
Chapter 4: LSC Simulation Characterization

4.1 – Simulation Precision

Before beginning a Monte Carlo simulation, it is important to understand how many realizations are necessary to obtain precise results such that, if the simulation is run multiple times under the same conditions, the same result is obtained within reasonable error. Additionally, since total CPU load and solution time is proportional to the number of realizations, it is desirable to minimize the number of realizations required to obtain a precise result to reduce the time it takes to run a simulation. Due to various assumptions made in the model and real-world variance that occurs within material qualities and manufacturing tolerances, a relative standard deviation (relative standard error within ±σ) of about ±2% should be more than sufficient for this model.

To determine the number of realizations required to obtain a result that is precise within ±2% relative standard error, \( \eta_{PCE} \) was evaluated 50 times each for 1000, 2500, 5000, 10000, 25000, 50000, 100000, and 250000 realizations as shown in figure 27, using a typical LSC configuration comprised of Si solar cells attached to a 300×300×3 mm³ PMMA waveguide filled with 200μM of Red305 dye.

![Figure 27: A plot of ηPCE vs. # of realizations for 1000, 2500, 5000, 10000, 25000, 50000, 100000, and 250000 realizations. A total of 50 simulations were performed at each number of realizations.](image)

Using the data at each realization number, standard deviation, mean, median, relative standard deviation, and time per realization were calculated as shown in table 1.
Table 1: Statistical data representing the precision and solution time per realization required to run a simulation using a various number of realizations (solar photons generated).

<table>
<thead>
<tr>
<th>Realizations</th>
<th>STDEV</th>
<th>AVG</th>
<th>MED</th>
<th>%RSD</th>
<th>TIME / Sim</th>
</tr>
</thead>
<tbody>
<tr>
<td>1,000</td>
<td>0.294367</td>
<td>2.290446</td>
<td>2.25098</td>
<td>12.85%</td>
<td>0:00:01</td>
</tr>
<tr>
<td>2,500</td>
<td>0.196538</td>
<td>2.309255</td>
<td>2.35461</td>
<td>8.51%</td>
<td>0:00:03</td>
</tr>
<tr>
<td>5,000</td>
<td>0.121204</td>
<td>2.270751</td>
<td>2.24665</td>
<td>5.34%</td>
<td>0:00:07</td>
</tr>
<tr>
<td>10,000</td>
<td>0.084313</td>
<td>2.286752</td>
<td>2.27686</td>
<td>3.69%</td>
<td>0:00:15</td>
</tr>
<tr>
<td>25,000</td>
<td>0.059828</td>
<td>2.293817</td>
<td>2.29094</td>
<td>2.61%</td>
<td>0:00:40</td>
</tr>
<tr>
<td>50,000</td>
<td>0.041308</td>
<td>2.285695</td>
<td>2.28377</td>
<td>1.81%</td>
<td>0:01:24</td>
</tr>
<tr>
<td>100,000</td>
<td>0.030042</td>
<td>2.297853</td>
<td>2.29845</td>
<td>1.31%</td>
<td>0:02:46</td>
</tr>
<tr>
<td>250,000</td>
<td>0.013807</td>
<td>2.293481</td>
<td>2.29327</td>
<td>0.60%</td>
<td>0:06:45</td>
</tr>
<tr>
<td>500,000</td>
<td>0.011926</td>
<td>2.293093</td>
<td>2.29353</td>
<td>0.52%</td>
<td>0:12:34</td>
</tr>
</tbody>
</table>

Data from table 1 for relative standard deviation (%RSD) and solution time per simulation (TIME / Sim) are plotted in figure 28. To obtain the specific number of realizations required to obtain relative standard deviations of 2.0%, 1.0%, and 0.5%, fitting functions were generated from the plot.

Figure 28: A plot of relative standard deviation and solution time per simulation vs. # of realizations derived from table 1. With respect to # of realizations, relative standard deviation displays a power law relationship, and solution time per simulation displays a linear relationship.

Based on the fitting functions generated from the plot in figure 28, the number of realizations required to obtain relative standard deviation values of 2.0%, 1.0%, 0.5%, and 0.25% are nearly 40000, 150000, 540000, and 2000000 which are expected to take 1min 5sec, 3min 53sec, 13min 46 sec, and 50min 50sec per simulation respectively. Using between 40000 and 150000 realizations per simulation should be sufficient to obtain a reasonable balance between precision and solution time.
4.2 – Simulation Accuracy

To analyze the accuracy and reliability of the LSC Monte Carlo ray-tracing simulation, real-world LSC data must be compared to results from the simulation. Experimental data was obtained from various sources of literature and compared to results obtained using the same materials and parameters in the LSC simulation developed for this thesis. If the results differ significantly, the validity of the assumptions made in the model must be scrutinized.

4.2.1 – Red305 Organic Dye LSC Analysis

The current world record single LSC efficiency is held by Sloof et al. published in their 2008 paper “A Luminescent Solar Concentrator with 7.1% Power Conversion Efficiency” [22]. This conversion efficiency was achieved by doping small 5×5×0.5 cm³ PMMA sheets with two organic dyes known as Lumogen® F-Red305 (developed by BASF Corporation) and Flourescence Yellow CRS040 (developed by Radiant Color), coupling the LSC to high efficiency FhG-ISC GaAs solar cells, and adding a diffuse air-gap BSR with a reflectance of 0.97. Data obtained for an identical LSC material system without the addition of a BSR yielded \( \eta_{PCE} \) of 5.3% when all 4 GaAs solar cells were connected in parallel. The concentrations of Red305 and CRS040 used in the study were 0.01wt% and 0.003wt% respectively. Figure 29 shows the absorption spectrum and normalized emission spectrum of Red305 (adapted from [40]) at a concentration of 30μM and path length of 5mm, as well as the EQE(\( \lambda \)) curve of a GaAs solar cell (adapted from [55]) and the normalized AM1.5G solar spectrum.

![BASF Lumogen® F-Red 305](image)

**Figure 29:** Absorption spectrum and normalized emission spectrum of BASF Lumogen F-Red 305 organic dye in PMMA at a concentration of 30μM and optical path length of 5mm. The the EQE(\( \lambda \)) curve of a GaAs solar cell and the normalized AM1.5G spectral photon irradiance are also shown to compare how well they overlap with the Red305 emission and absorption spectrum respectively.
In the study by Sloof et al., the concentrations of the fluorescent materials are reported in units of wt%. Since the LSC simulation requires molar concentration units, the wt% concentration of Red305 was converted to molar units using the following equation.

\[
c_x = \frac{\rho_{wg}(\text{wt}\%)_{fm}}{M_{fm}}
\]

where \((\text{wt}\%)_{fm}\) is the wt% concentration of the fluorescent material, \(\rho_{wg}\) is the density of the waveguide, and \(M_{fm}\) is the molar mass of the fluorescent material. This equation assumes that the total mass of the fluorescent material is negligible relative to the total mass of the waveguide. The density of PMMA is about 1.18g/cm³, and the molar mass of Red305 is 1078g/mol; thus the molar concentration \((M \equiv \text{mol/L})\) of Red305 is 109.5μM.

Red305 is one of the most commonly studied fluorescent materials in LSC designs due to its extremely high \(\eta_{QY}\) around 0.98, relatively broad absorption spectrum, relatively minor absorption/emission spectrum overlap, and high stability [56]. In conventional LSC designs, Red305 has proven itself to be one of the most efficient and reliable fluorescent materials; thus, it is often used as a benchmark for other fluorescent materials. Since detailed plots of the absorption and emission spectra of CRS040 could not be found, the wt% concentration of CRS040 is less than a 1/3 of the wt% concentration of Red305, and the Monte Carlo simulation developed for this paper does not have functionality to incorporate more than one dye into each LSC, the simulation model was simplified to only use Red305 dye. Since Red305 is the primary system dye, and other research has shown the addition of an optimum amount of CRS040 to Red305 typically only improves \(I_{SC}\) by ~10% [56], the efficiency results of the simulation should be similar to but only approximately 10% lower than experimental results. If \(I_{SC}\) is reduced by about 10% and the superposition assumption is true, \(V_{OC}\) of the simulation results relative to the experimental results should reduce by roughly \((nkT/q) \times \ln(0.9)\), which is negligibly small but should be ~0.003V or greater depending on \(n\) of the solar cell.

In the following results, 100,000 photons were modeled to simulate the material system used in the the paper by Sloof et al., sans 0.003wt% CRS040 dye. Table 2 shows data extracted from the paper by Sloof et al. compared to simulation results.

<table>
<thead>
<tr>
<th>Source</th>
<th>Dim. (mm³)</th>
<th>G</th>
<th>Fluor. Mat. 1</th>
<th>Fluor. Mat. 2</th>
<th>(I_{SC}) (mA)</th>
<th>(V_{OC}) (V)</th>
<th>FF</th>
<th>(\eta_{PCE})</th>
<th>(F_{PCE})</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exp.</td>
<td>50×50×5</td>
<td>2.5</td>
<td>0.01wt% Red305</td>
<td>0.003wt% CRS040</td>
<td>174</td>
<td>0.997</td>
<td>0.768</td>
<td>5.30%</td>
<td>0.57</td>
</tr>
<tr>
<td>Sim.</td>
<td>50×50×5</td>
<td>2.5</td>
<td>None</td>
<td>0.01wt% Red305</td>
<td>166.4</td>
<td>0.987</td>
<td>0.83</td>
<td>5.46%</td>
<td>0.59</td>
</tr>
</tbody>
</table>

Table 2: A comparison between experimental [22] and simulated results for a 50×50×5 mm³ LSC using a PMMA waveguide, Red305 dye, and GaAs solar cells connected in parallel.
Interestingly, the $I_{SC}$ and $V_{OC}$ produced by the simulated LSC are 4.4% and 0.01% worse than experimental results, as expected, but the simulated $\eta_{PCE}$ is actually 3.0% higher relative to experimental results, which is not expected. This error stems from the 8.1% difference in FF between simulated and experimental data. The cause of this discrepancy can be understood based on the assumptions made in the LSC simulation. In the simulation, it is assumed that FF will remain constant. The experimentally determined FF of the GaAs solar cells used in the research by Sloof et al. are explicitly stated as being 0.83 when exposed to AM1.5 sunlight, which is the same value used in the LSC simulation. However, it can be seen in table 1 that the experimentally determined FF of the GaAs solar cell attached to the Red305-CRS040 LSC is only 0.768. The values obtained for $F_{opt}$, $F_{opt}'$, and $F_{PCE}$ in the simulation are 0.26, 0.34, and 0.59 respectively. Therefore, the LSC fabricated in the study by Sloof et al. is actually functioning as a solar diffuser rather than a solar concentrator; a common problem among many research articles that claim high efficiency results.

Although the FF assumption proves to be slightly inaccurate in this case, it is likely that a GaAs p-n junction solar cell will exhibit diode behavior such that the superposition assumption used to calculate $I_{SC}$ and $V_{OC}$ is reasonably valid. Recalculating the simulated $\eta_{PCE}$ by assuming $FF \sim 0.76$ instead of 0.83 yields $\eta_{PCE} = 5.0\%$, which is an extremely reasonable value to expect considering CRS040 dye was removed from the system.

### 4.2.2 – PbS and CdSe/ZnS Quantum Dot LSC Analysis

A recent article published by Shcherbatyuk et al. titled “Viability of using near infrared PbS quantum dots as active materials in luminescent solar concentrators” [39] studied the use of PbS and CdSe/ZnS QDs in LSCs due to their extremely broad absorption spectrum, good $\eta_{QY}$, and emission spectrum that couples well to Si solar cells. Using PbS and CdSe/ZnS QDs purchased from Evident Technologies, Shcherbatyuk et al. constructed solution based LSCs encased in quartz panels with dimensions of $45 \times 12 \times 4 \text{mm}^3$ and an optical path length of 2mm. Silicon solar cells with an active width of 3mm were attached to the edges of the panel to measure the optical and power conversion efficiencies of the device.

It was determined that using a PbS QD concentration of 193$\mu$M and CdSe/ZnS QD concentration of $\sim$3.5$\mu$M yielded the highest optical and power conversion efficiencies for the panel dimensions used. Although the paper claims that $G = 11$ in their samples, this geometric gain is referenced from only one small edge of the LSC. By attaching PV cells with an active width of 3mm to all four edges, $G$ of the entire LSC system is only about 1.58. Figure 30 shows the absorption spectrum and normalized emission spectrum of PbS QDs and CdSe/ZnS QDs in toluene at a concentration of 193$\mu$M and 3.5$\mu$M respectively (adapted from [39]) with an optical path length of 2mm, as well as the EQE($\lambda$) curve of a Si solar cell (adapted from [57]) and the normalized AM1.5G solar spectrum.
Figure 30: Absorption spectrum and normalized emission spectrum of PbS and CdSe/ZnS quantum dots [39] in toluene at concentrations of 193μM and 3.5 μM respectively with an optical path length of 2mm. The EQE(λ) curve of an ultra-high efficiency Sunpower mono-crystalline silicon (C-Si) solar cell [57] and the normalized AM1.5G spectral photon irradiance are also shown to compare how well they overlap with the emission and absorption spectrum of the quantum dots respectively.

To simulate the LSC system characterized by Shcherbatyuk et al., some assumptions need to be made. First, to model the effects of using a 4mm thick quartz panel with a 2mm optical path length, the simulated LSC dimensions are 45×12×4mm³, and the concentration of the fluorescent material is halved to account for both the doubling of the optical path length in the simulation and the 1mm thickness on the top and bottom of the quartz panel that light is able to propagate through without encountering QDs. To model the effects of using 3mm wide solar cells over a 4mm edge thickness, the η_{opt}^ε and η_{PCE} obtained in the simulation results are multiplied by a correction factor of 0.75 to account for the 1mm thick area around the edges that is not covered by solar cells, which reduces I_{SC}, I_{PV}, and A_{PV} by 1/4.

Though the properties and make of the Si solar cells attached to the edges are not listed in the article, an approximate value of the solar cell efficiency was extracted from the experimental results. Given that η_{opt}^ε is the ratio of the short-circuit current generated in the PV cells attached to the LSC in sunlight and the short-circuit current generated in the PV cells with a front surface area of A_{LSC} in sunlight, η_{PCE} can be approximated by the product of η_{opt}^ε and η_{PV}; thus, η_{PV} can be estimated well by the ratio of η_{PCE} and η_{opt}^ε. In the study, it is given that 193μM PbS QDs and ~3.5μM CdSe/ZnS QDs produce η_{PCE} of 3.2% and 1.2% and η_{opt}^ε of 12.6% and 4.5% respectively. Using the data for PbS QDs and CdSe/ZnS QDs, η_{PV} is estimated to be 25.4% and 26.6% respectively. These values are unrealistically high for a silicon solar cell because the world record efficiency is about 25%. Therefore, it must be true that V_{OC} and/or FF of the Si solar cell is higher under LSC edge illumination than AM1.5 solar illumination.
It is important to note that, with $\eta_{opt}^{\xi}$ of 12.6% and $G$ of ~1.58, the current concentration ratio $I_{SC}/I_{PV}$ of the PbS QD LSC system is only ~20%. Thus, once again, the experimentally characterized LSC is actually acting as a solar diffuser rather than a solar concentrator because the current generated in the solar cells attached to the LSC is only 20% of the current that would be generated if the solar cells were exposed directly to sunlight. If the superposition assumption is assumed to be reasonably valid for the Si solar cell used in this experimental work, $V_{OC}$ of the solar cells attached to the LSC relative to $V_{OC}$ of the solar cells in direct sunlight should be reduced by roughly $(nkT/q) \cdot \ln(0.20)$, i.e. ~0.04V or greater depending on $n$ of the solar cell. Thus, it can be reasonably concluded that there must be a substantial increase in $FF$ of the PV cell when it is illuminated under LSC edge illumination relative to solar illumination.

Due to the fact that $I_{SC}$, $V_{OC}$, and $FF$ of the experimentally characterized Si solar cells are not provided in the paper, and the authors of the paper have currently not responded to emails inquiring about the matter, whether or not the hypotheses posed in this section about the nature of the Si solar cells used in the study cannot be validated. Regardless, since $FF$ is expected to increase under LSC edge illumination relative to solar illumination, resulting in effective $\eta_{PV}$ values between 25.4% and 26.6%, simulation results for a simulated Sunpower Si solar cell with $\eta_{PV} \equiv 24.2\%$ should provide slightly lower $\eta_{PCE}$ than experimental results since $FF$ is assumed to be constant in the simulation. However, $\eta_{opt}^{\xi}$ should be similar to experimental results since it depends primarily on the optical properties of the LSC.

In the following results, 100,000 photons were simulated to model the PbS QD material system used in the study. However, the simulation results need to be modified to correlate with the way several variables are defined in the study. In the study done by Shcherbatyuk et al., absorption efficiency is defined as the fraction of incident photons with wavelengths below the cutoff wavelength of the solar cell absorber material ($\lambda_c$) that are absorbed by the fluorescent material, which will be referred to as $\eta_{abs}^{\lambda_c}$. About 64% of the total incident photon flux consists of photons with wavelengths below the cutoff wavelength of Si. Thus, $\eta_{abs}$ determined in the simulation, which is integrated over the entire solar spectrum, can be divided by 0.64 to obtain $\eta_{abs}^{\lambda_c}$. Optical efficiency is the electronic optical efficiency defined in section 2.7.1. Finally, a loss term defined in the study as $\eta_L$ represents losses due to self-absorption and escape-cone loss which is determined using equation 60.

$$\eta_L = 1 - \frac{\eta_{opt}^{\xi}}{\eta_{abs}^{\lambda_c} \eta_{QY}} \quad (60)$$

Table 3 shows data extracted from the paper by Shcherbatyuk et al. compared to simulation results for PbS QD and CdSe/ZnS QD LSCs. The dimensions of the waveguide and the concentration of the fluorescent material are modified from the experimental study to appropriately model an LSC where only half of the waveguide thickness contains fluorescent material.
Table 3: A comparison between experimental [39] and simulated results for 45×12×4 mm³ (G = 1.6) LSCs using glass waveguides, PbSe or CdSe/ZnS quantum dots, and Si solar cells.

<table>
<thead>
<tr>
<th>Source</th>
<th>Dim. (mm³)</th>
<th>G</th>
<th>Fluor Mat.</th>
<th>cₓ (μM)</th>
<th>ηQY</th>
<th>λc</th>
<th>ηabs</th>
<th>ηL</th>
<th>ηopt</th>
<th>ηPCE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exp.</td>
<td>45×12×4(2)†</td>
<td>1.6</td>
<td>PbS QDs</td>
<td>193</td>
<td>0.30</td>
<td>-0.70</td>
<td>~0.40</td>
<td>12.6%</td>
<td>3.2%</td>
<td></td>
</tr>
<tr>
<td>Sim.</td>
<td>45×12×4†2</td>
<td>1.6</td>
<td>PbS QDs</td>
<td>96.5†2</td>
<td>0.30</td>
<td>-0.66</td>
<td>~0.64</td>
<td>7.1%</td>
<td>1.6%</td>
<td></td>
</tr>
<tr>
<td>Sim.</td>
<td>45×12×4†2</td>
<td>1.6</td>
<td>PbS QDs</td>
<td>96.5†2</td>
<td>0.49</td>
<td>-0.66</td>
<td>~0.61</td>
<td>12.7%</td>
<td>2.9%</td>
<td></td>
</tr>
<tr>
<td>Exp.</td>
<td>45×12×4(2)†</td>
<td>1.6</td>
<td>CdSe QDs</td>
<td>3.50</td>
<td>0.50</td>
<td>-0.22</td>
<td>~0.59</td>
<td>4.5%</td>
<td>1.2%</td>
<td></td>
</tr>
<tr>
<td>Sim.</td>
<td>45×12×4†2</td>
<td>1.6</td>
<td>CdSe QDs</td>
<td>1.75†2</td>
<td>0.50</td>
<td>-0.23</td>
<td>~0.59</td>
<td>4.7%</td>
<td>1.1%</td>
<td></td>
</tr>
</tbody>
</table>

† Waveguide thickness is 4mm, but the optical path thickness is only 2mm
†2 Waveguide thickness and optical path length are simulated as 4mm, but to account for the true 2mm optical path length, the fluorescent material concentration is halved in the simulation.
†3 The loss term ηL was calculated using the efficiency values listed in the paper, but the calculated values based on the reported efficiencies of PbS QD and CdSe/ZnS QD conflict with the values for ηL reported in the study.

At first glance, the simulation results for PbS QDs match very poorly, whereas the simulation results for CdSe/ZnS QDs match very well with experimental results. The simulation results for PbS QDs with ηQY of 0.30 provide ηopt and ηPCE values of nearly 1/2 of the experimentally obtained values. It is interesting to note that a reasonable maximum value for ηopt if no self-absorption is present and the PV cells only cover ¾ of the edge thickness is equal to the product of ηabs, ~0.70, ηtrap, ~0.75, ηQY ~0.30, and the correction factor of 0.75, which turns out to be ~11.8%. Furthermore, as seen in figure 25, there is a significant degree of overlap between the absorption and the emission spectrum of PbS QDs. Thus, a large amount of self-absorption should be expected, which will further reduce ηopt. This simple analysis provides evidence that ηopt should not be larger than 12% for PbS QDs with ηQY of only 0.3. It is also interesting to note that the authors reported that ηL of PbS QD LSCs only increases by 3% (relative) from 50μM to 193μM solution concentration. Due to the degree of overlap between the absorption and emission spectra of PbS QDs, the miniscule magnitude of difference in ηL for such a large concentration difference is an unreasonable result.

It is not uncommon to see PbS QDs with ηQY as high as 0.8, especially for relatively small QDs [25]. Since the authors did not mention any information about measurements or confirmation of the supposed ηQY values obtained from the vendor, the likely cause of the discrepancy between the experimentally obtained values from the study and the simulated results stems from incorrectly assumed ηQY reported in the study. After amending ηQY in the simulation, it was discovered that PbS QDs with ηQY of 0.49 yielded results that correspond well with the experimentally determined value of ηopt, but ηPCE still differed by about 9.4% (relative) which was expected due to the assumed characteristics of the Si PV in addition to the fact that FF is assumed to be constant.
Chapter 5: Infrared Emitting PbSe Quantum Dot LSCs

5.1 – Introduction and Purpose

Research on QD LSCs in the past has primarily focused on visible emitting QD materials such as CdSe/ZnS, but efficiency of a visible-emitting LSC is limited by the lack of infrared photon absorption. To this date, PbSe QDs have not been studied as the active fluorescent material in LSC devices. This is likely due to the fact that typical PbSe QD emission wavelengths fall beyond the absorption range of Si PV cells. In a PbSe QD LSC, germanium (Ge) is the most likely PV absorber material due to its band-gap energy of 0.67eV and cutoff wavelength near 1850nm. The present record photovoltaic power conversion efficiency ($\eta_{PV}$) for a stand-alone Ge solar cell is about 7.9% under AM1.5G sunlight [58]. Although the efficiency of Ge solar cells is relatively low compared to Si and GaAs solar cells, it is worthwhile to investigate the use of PbSe QDs in LSCs due to their broadband absorption spectrum and infrared absorption/emission characteristics. Tandem LSC configurations, which utilize stacks of LSCs with different fluorescent materials to maximize $\eta_{PCE}$ may benefit from the addition of a PbSe QD LSC layer to harvest infrared photons.

5.2 – PbSe QD Characterization

The PbSe QDs used to model the absorption and emission spectra were fabricated in-house by preparation methods similar to that of Yu et al. [36] with resulting absorption and emission peaks at 1465nm and 1515nm respectively. Figure 31 shows a photograph of PbSe QDs fabricated for this research and a plot of the absorption spectra and normalized emission spectrum of PbSe QDs for $c = 0.35, 1.1, 5.3, \text{and } 39.6\mu M$.

**Figure 31:** On the left, a small bottle of highly concentrated infrared emitting PbSe quantum dots. The On the right, the absorption spectra (percent absorption vs. wavelength) at QD solution concentrations of 0.35μM, 1.1μM, 5.3μM and 39.6μM and emission spectrum (normalized photoluminescence intensity vs. wavelength) of PbSe QDs in a 5mm thick container.
The absorption spectra of PbSe QDs dispersed in tetrachloroethylene were measured with a Perkin Elmer UV-VIS-NIR spectrometer to obtain percent absorption vs. wavelength curves for a 5mm thick sample. The emission spectrum was measured using a Spectral Products CM110 monochromator and a Stanford Research Systems SR810 lock-in detector coupled to a chopper operating at 400Hz. A 615nm laser was used as the photo-excitation source, and photoluminescence (PL) output was channeled to a fiber optic cable located directly adjacent to the laser-excited QDs in a 45×12×4 mm³ glass container.

The large overlap between the absorption and emission spectra causes significant self-absorption at high solution concentrations. One way of characterizing self-absorption and the degree of absorption/emission spectrum overlap is through PL red-shift analysis [38], [39]. Due to the band-gaps and size-dispersion of QDs in the system, larger, lower energy emitting QDs can reabsorb light emitted by smaller, higher energy emitting QDs, but not vice versa. Figure 32 shows a plot of normalized PL intensity vs. wavelength for excitation-to-detector distance \( d \) for \( d = 0, 1.0, 2.2, 3.5, \) and 4.2cm, and a schematic of the experimental setup for collecting the red-shifted emission curve.

![Excitation-to-Detector Distance](image)

**Figure 32:** (left) PL red-shift measured at excitation-to-detector distances, \( d \), for \( d = 0, 1.0, 2.2, 3.5, \) and 4.2cm. (right) Schematic of the red-shift measurement setup; the optical path length is varied by changing the excitation-to-detector distance, \( d \).

Red-shifted PL spectra are obtained by increasing the optical path length of photons traveling through the LSC. Thus, red-shifted emission spectra were obtained by varying the distance, \( d \), between the laser excitation point and the fiber-optic cable located at the edge of the sealed 45×12×4 mm³ glass container. Increasing \( d \) from 0cm to 4.2cm caused the peak PL intensity to shift from 1515nm to 1620nm. The 105nm shift is evidence of significant self-absorption loss for emitted photons with wavelengths less than ~1600nm.
5.3 – Monte Carlo Study

Monte Carlo simulations were performed to evaluate the efficiencies and losses of PbSe QD LSCs with various QD concentrations and LSC thicknesses. The PV cells attached to the edges were modeled based on Ge thermo-photovoltaic (TPV) cells, which have enhanced QE at extended wavelengths in the IR spectrum relative to conventional Ge PV cells. Figure 33 shows the absorption spectrum and normalized emission spectrum of PbSe QDs and in tetrachloroethylene at a concentration of 3μM with an optical path length of 5mm, as well as the EQE(λ) curve of a Ge TPV solar cell (adapted from [58]) and the normalized AM1.5G solar spectrum.

![PbSe Quantum Dots](image)

**Figure 33:** Absorption spectrum and normalized emission spectrum of PbSe quantum dots in tetrachloroethylene at a concentration of 3μM and optical path length of 5mm. The EQE(λ) curve of a Ge TPV cell specifically tailored to long photon wavelengths in the IR spectrum and the normalized AM1.5G spectral photon irradiance are also shown to compare how well they overlap with the emission and absorption spectrum of the quantum dots respectively.

The front surface area of all the simulated LSCs in the following sub-section were chosen to be 300×300 mm² as this represents a realistic size for a small, usable LSC. The η_QV of high-quality PbSe QDs is often reported to be higher than 80% when fluorescence characterization is accomplished using comparison techniques with other known infrared-emitters such as IR-125 and IR-26 [26], [36]. However, according to fluorescence data collected using integrating sphere [37], η_QV of 40% is an optimistic value for PbSe QDs with band gaps smaller than 1.1eV. For comparison and completeness, two sets of PbSe QDs will be modeled in this simulation with η_QV of 40% and 80% respectively. In the following results, 50,000 solar photons were generated in each simulation.
5.3.1 - Simulation Results

The first step necessary to characterize a fluorescent material in an LSC is to determine the fraction of absorbed photons, \( \eta_{abs} \), as a function of concentration and thickness. Due to the extremely broad absorption spectrum of PbSe QDs that spans well into the infrared spectrum, it’s reasonable to expect that they are capable of displaying \( \eta_{abs} \) larger than any other visible or NIR emitting fluorescent materials that have been previously studied. Figure 34 shows a plot of absorption efficiency (\( \eta_{abs} \)) vs. PbSe QD solution concentration (\( c_x \)) for \( c_x \) ranging from 0.125 to 40\( \mu \)M and \( t = 2.5, 5, \) and 10mm. As expected, PbSe QDs display exceptional \( \eta_{abs} \) values due to their broad absorption spectrum spanning the entire visible spectrum and infrared spectrum up to ~1600nm. Also, as expected, thicker LSCs yield greater \( \eta_{abs} \) due to the longer optical absorption path length. However, the concentration capabilities of an LSC reduce as \( t \) increases due to a corresponding reduction of \( G \), so it is not necessarily advantageous to use a thicker LSC to attain higher \( \eta_{abs} \).

![Figure 34: Absorption efficiency (\( \eta_{abs} \)) vs. PbSe QD concentration (\( c \)) for simulated 2.5, 5.0, and 10mm thick LSCs with \( c \) ranging from 0.1 to 50\( \mu \)M.](image)

Although superior absorption efficiencies are obtained at higher PbSe QD concentrations, the incidence of self-absorption increases as concentration increases. Therefore, it is always necessary to balance \( \eta_{abs} \) with \( \eta_{SA} \) in any LSC system to obtain the highest possible \( \eta_{opt} \) and \( \eta_{PCE} \). Figure 35 shows a plot of self-absorption efficiency vs. concentration for 300\( \times \)300\( \times \)2.5 mm\(^3\) PbSe QD LSCs with \( \eta_{QY} \) of 0.40 and 0.80. Self-absorption efficiency results for 5mm and 10mm thick LSCs are very similar to that of 2.5mm thick LSCs.
Figure 35: Self-absorption efficiency ($\eta_{SA}$) vs. PbSe QD concentration ($c$) for simulated 300×300×2.5 mm$^3$ LSCs with $c$ ranging from 0.1 to 50μM and $\eta_{QY} = 0.40$ and 0.80.

As expected, self-absorption efficiency is substantially better for PbSe QDs with higher $\eta_{QY}$ and at lower PbSe QD concentrations. The average optical path length to an edge is dependent on length and width of the LSC, but not thickness. Therefore, self-absorption efficiency is relatively independent of LSC thickness, but strongly dependent on the length and width of an LSC. Since $\eta_{QY}$ and $\eta_{\text{trap}}$ are constant in an LSC system and $\eta_{\text{opt}}$ can be expressed as the product of $\eta_{\text{abs}}, \eta_{QY}, \eta_{\text{trap}},$ and $\eta_{SA}$, optical efficiency is maximum at the concentration where the product of $\eta_{\text{abs}}$ and $\eta_{SA}$ is maximized. Figure 36 shows plots of optical efficiency vs. solution concentration for simulated 300×300×2.5 mm$^3$, 300×300×5 mm$^3$, and 300×300×10 mm$^3$ PbSe QD LSCs with $\eta_{QY}$ of 0.40 and 0.80 and $c$ ranging from 0.1 to 50μM.

Figure 36: Optical efficiency ($\eta_{\text{opt}}$) vs. PbSe QD concentration ($c$) for simulated 300×300×2.5 mm$^3$, 300×300×5 mm$^3$, and 300×300×10 mm$^3$ LSCs with $c$ ranging from 0.1 to 50μM, and $\eta_{QY}$ of (a) 0.40 and (b) 0.80.
As seen in figure 34 (a) and (b), optical efficiency is strongly dependent on $\eta_{QY}$, solution concentration, and thickness. The optimal solution concentration shifts down as $t_{LSC}$ increases due to the dependency of optical absorption path-length on $t_{LSC}$. If the optical path length to absorb solar photons is longer, the necessary concentration to absorb a specified fraction of incident photons reduces. Thus, $\eta_{opt}$ is improved by reducing the fluorescent material concentration to reduce the incidence of self-absorption. The optimal solution concentration shifts up as $t_{LSC}$ increases due to the fact, even though the incidence of self-absorption is dictated by the fluorescent material concentration, the magnitude of self-absorption loss is dictated. Thus, at higher $t_{LSC}$, the LSC system can sustain a higher level of self-absorption without incurring as much loss. Table 4 shows results for various simulated PbSe QD LSCs with $A_{LSC} = 300 \times 300 \text{mm}^2$ at optimized QD concentrations for highest efficiency. Germanium TPV cells [58] with 6.3% AM1.5 photovoltaic power conversion efficiency were modeled to determine the electrical output, power conversion efficiency, and flux gain of simulated PbSe QD LSCs due to their excellent long wavelength response.

Table 4: LSC Monte Carlo simulation results for PbSe QD LSCs with and without specular back-surface reflectors for $A_{LSC}=300 \times 300 \text{mm}^2$ and optimized QD concentrations.

<table>
<thead>
<tr>
<th>t (mm)</th>
<th>G</th>
<th>BSR</th>
<th>$c_x$ (μM)</th>
<th>$\eta_{QY}$</th>
<th>$\eta_{opt}$</th>
<th>$\eta_{PCE}$</th>
<th>$F_{PCE}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.5</td>
<td>30</td>
<td>No</td>
<td>2.4</td>
<td>0.40</td>
<td>2.63%</td>
<td>0.18%</td>
<td>1.01</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Yes</td>
<td>1.6</td>
<td>0.40</td>
<td>3.66%</td>
<td>0.27%</td>
<td>1.49</td>
</tr>
<tr>
<td></td>
<td></td>
<td>No</td>
<td>3.5</td>
<td>0.80</td>
<td>8.32%</td>
<td>0.63%</td>
<td>3.49</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Yes</td>
<td>2.2</td>
<td>0.80</td>
<td>11.1%</td>
<td>0.90%</td>
<td>5.03</td>
</tr>
<tr>
<td>5.0</td>
<td>15</td>
<td>No</td>
<td>1.5</td>
<td>0.40</td>
<td>3.76%</td>
<td>0.26%</td>
<td>0.73</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Yes</td>
<td>1.0</td>
<td>0.40</td>
<td>5.09%</td>
<td>0.37%</td>
<td>1.03</td>
</tr>
<tr>
<td></td>
<td></td>
<td>No</td>
<td>2.3</td>
<td>0.80</td>
<td>11.3%</td>
<td>0.83%</td>
<td>2.33</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Yes</td>
<td>1.2</td>
<td>0.80</td>
<td>14.6%</td>
<td>1.16%</td>
<td>3.28</td>
</tr>
<tr>
<td>10</td>
<td>7.5</td>
<td>No</td>
<td>0.7</td>
<td>0.40</td>
<td>5.07%</td>
<td>0.34%</td>
<td>0.48</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Yes</td>
<td>0.5</td>
<td>0.40</td>
<td>7.11%</td>
<td>0.52%</td>
<td>0.72</td>
</tr>
<tr>
<td></td>
<td></td>
<td>No</td>
<td>1.4</td>
<td>0.80</td>
<td>14.6%</td>
<td>1.08%</td>
<td>1.51</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Yes</td>
<td>0.8</td>
<td>0.80</td>
<td>18.5%</td>
<td>1.48%</td>
<td>2.07</td>
</tr>
</tbody>
</table>

PbSe QDs with $\eta_{QY}$ of 0.40 cannot function well as the fluorescent material for LSCs at the specified dimensions. For all configurations listed with $\eta_{QY}$ of 0.40 in Table 1, $F_{PCE}$ is less than 1.5 and $\eta_{PCE}$ is less than 0.55%. If $F_{PCE}$ is less than 1, the Ge TPV cells attached to the PbSe QD LSC would actually produce more power if they were removed and placed in direct sunlight; i.e. the LSC would be effectively functioning as a luminescent solar diffuser. The combination of extreme NRR loss and self absorption, coupled with a relatively low efficiency PV cell results in extremely low device efficiency.
On the other hand, PbSe QDs with $\eta_{QY}$ of 0.80 function relatively well as the fluorescent material for LSCs at the specified dimensions, albeit with low $\eta_{PCE}$. For all the simulated LSCs with optimized concentrations and $\eta_{QY}$ of 0.80, $F_{PCE}$ is greater than 1. Therefore, these LSCs are functioning effectively as solar concentrators. Furthermore, simulation results show that the addition of a specular BSR to a PbSe QD LSC can boost $\eta_{PCE}$ above 1.0% while simultaneously improving $F_{PCE}$. The addition of a BSR is particularly effective in PbSe QD LSCs due to the high incidence of self absorption. Since the addition of a BSR effectively doubles the solar absorption path length, self-absorption loss can be reduced while solar absorption characteristics are maintained by reducing the fluorescent material concentration.

5.3.2 – Tandem LSC Results

In addition to single LSC configurations, PbSe QD LSCs can also be used in tandem concentrator configurations to improve LSC efficiencies by collecting infrared photons that cannot be harvested by conventional, visible-emitting LSCs. Tandem LSCs were simulated using Lumogen® F Red305 dye in the top LSC coupled to c-Si PV cells, and PbSe QDs with $\eta_{QY}$ of 0.8 in the bottom LSC coupled to Ge TPV cells. For LSCs to act in tandem electrically as well as optically, the solar cells between the two LSCs will either need to be connected in parallel or series, resulting in losses if voltage or current are not matched respectively. Although $I_{sc}$, $V_{oc}$, and FF are simulated for each cell at each edge, the IV curves are not. Thus, the tandem LSCs cannot be designed to match current or voltage at their respective operating points using this software. Table 5 shows results from Red305/PbSeQD tandem LSC simulations.

<table>
<thead>
<tr>
<th>Dim. ($\text{mm}^3$)</th>
<th>PV</th>
<th>Config.</th>
<th>BSR</th>
<th>Fluor. Mater.</th>
<th>$c$ (μM)</th>
<th>$\eta_{QY}$ (%)</th>
<th>$\eta_{opt}$ (%)</th>
<th>$\eta_{PCE}$ (%)</th>
<th>$F_{PCE}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>300×300×2.5 c-Si</td>
<td>Single</td>
<td>No</td>
<td>Red305</td>
<td>200</td>
<td>0.98</td>
<td>7.56</td>
<td>2.57</td>
<td>4.68</td>
<td></td>
</tr>
<tr>
<td>300×300×2.5 c-Si</td>
<td>Single</td>
<td>Yes</td>
<td>Red305</td>
<td>200</td>
<td>0.98</td>
<td>9.68</td>
<td>3.30</td>
<td>6.02</td>
<td></td>
</tr>
<tr>
<td>300×300×2.5 c-Si</td>
<td>Tandem</td>
<td>No</td>
<td>Red305</td>
<td>200</td>
<td>0.98</td>
<td>7.63</td>
<td>2.59</td>
<td>4.72</td>
<td></td>
</tr>
<tr>
<td>300×300×2.5 PbSe QD</td>
<td>4.3</td>
<td>0.80</td>
<td>6.20</td>
<td>0.44</td>
<td>2.17</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>300×300×2.5 Ge</td>
<td>Tandem</td>
<td>Yes</td>
<td>Red305</td>
<td>200</td>
<td>0.98</td>
<td>7.78</td>
<td>2.63</td>
<td>4.79</td>
<td></td>
</tr>
<tr>
<td>300×300×2.5 PbSe QD</td>
<td>2.6</td>
<td>0.80</td>
<td>8.82</td>
<td>0.67</td>
<td>3.38</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Simulation results suggest that, although PbSe QD LSCs retain more than 70% of their direct illumination efficiency, the addition of a BSR to a Red305 LSC is more advantageous than coupling it to a tandem PbSe QD LSC, even if the $\eta_{QY}$ of PbSe QDs is 0.80 and an additional BSR is added to the tandem LSC system. The additional cost of a specular BSR, at roughly $3/m^2$, should certainly be less than that of a PbSe QD LSC system. Thus, using a tandem PbSe QD LSC to harvest infrared radiation is not advisable unless the absorption and emission band overlap can be reduced and $\eta_{SA}$ can be improved.
5.3.3 – Quantum Dot LSC Comparison

Although the PbSe QD LSCs analyzed in the previous sub-section are modeled with $A_{LSC}$ of $300 \times 300 \text{ mm}^2$, front surface areas this large are typically not studied in experimental papers. Not only are LSCs with small front surface areas convenient to work with in a lab, they also deceptively improve LSC efficiencies by reducing the prevalence of self-absorption. As stated previously, LSC’s with small $A_{LSC}$ often cannot function effectively as solar concentrators due to the consequential reduction of $G$ with decreasing $A_{LSC}$. Nevertheless, it is interesting and noteworthy to compare experimental studies of small visible and NIR emitting QD LSCs to small simulated PbSe QD LSCs. Furthermore, it is also interesting to simulate visible and NIR emitting LSCs with larger $A_{LSC}$ to discover whether the fluorescent materials used in the experimentally characterized systems function as well as the authors’ assert. Table 6 shows a comparison between simulated CdSe/ZnS, PbS, and PbSe QD LSCs with small and large dimensions of $45 \times 12 \times 4 \text{ mm}^3$ and $300 \times 300 \times 2.5 \text{ mm}^3$ respectively. The small $A_{LSC}$ dimension is derived from the QD LSC paper by Shcherbytuk et al. discussed in section 4.1.2, for comparison with experimental results. However, in these simulations, the solar cells attached to the edges are assumed to have an active width that encompasses the entire LSC edge, thus reducing $G$ from ~1.6 to ~1.2, and boosting efficiencies by ~25% (relative). In the following results, 100,000 photons were generated for each simulation.

Table 6: A comparison between simulated CdSe/ZnS (CdSe), PbS, and PbSe QD LSCs with both large ($300 \times 300 \times 2.5 \text{ mm}^3 : G = 30$) and small ($45 \times 12 \times 4 \text{ mm}^3 : G = 1.2$) dimensions to evaluate the effects of size on LSC efficiency.

<table>
<thead>
<tr>
<th>Dim. (mm$^3$)</th>
<th>PV</th>
<th>QD</th>
<th>$c_x$ (μM)</th>
<th>$\eta_{QY}$</th>
<th>$\eta_{abs}$</th>
<th>$\eta_{SA}$</th>
<th>$\eta_{opt}$ (%)</th>
<th>$\eta_{opt}^\varepsilon$ (%)</th>
<th>$\eta_{PCE}$ (%)</th>
<th>$F_{PCE}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$45 \times 12 \times 4.0$</td>
<td>Ge</td>
<td>PbSe</td>
<td>14.0</td>
<td>0.80</td>
<td>.704</td>
<td>.685</td>
<td>28.7</td>
<td>35.3</td>
<td>1.89</td>
<td>0.41</td>
</tr>
<tr>
<td>$300 \times 300 \times 2.5$</td>
<td>Ge</td>
<td>PbSe</td>
<td>3.50</td>
<td>0.80</td>
<td>.403</td>
<td>.354</td>
<td>8.51</td>
<td>9.31</td>
<td>0.63</td>
<td>3.54</td>
</tr>
<tr>
<td>$45 \times 12 \times 4.0$</td>
<td>Si</td>
<td>PbS</td>
<td>96.5</td>
<td>0.49</td>
<td>.417</td>
<td>.707</td>
<td>10.7</td>
<td>12.9</td>
<td>3.94</td>
<td>1.20</td>
</tr>
<tr>
<td>$300 \times 300 \times 2.5$</td>
<td>Si</td>
<td>PbS</td>
<td>41.7</td>
<td>0.49</td>
<td>.253</td>
<td>.333</td>
<td>3.08</td>
<td>4.87</td>
<td>1.20</td>
<td>1.48</td>
</tr>
<tr>
<td>$45 \times 12 \times 4.0$</td>
<td>Si</td>
<td>CdSe</td>
<td>1.75</td>
<td>0.50</td>
<td>.145</td>
<td>.731</td>
<td>3.96</td>
<td>6.30</td>
<td>1.39</td>
<td>0.07</td>
</tr>
<tr>
<td>$300 \times 300 \times 2.5$</td>
<td>Si</td>
<td>CdSe</td>
<td>1.20</td>
<td>0.50</td>
<td>.086</td>
<td>.237</td>
<td>0.76</td>
<td>1.14</td>
<td>0.27</td>
<td>0.33</td>
</tr>
</tbody>
</table>

The $\eta_{opt}$ ratios between the large and small LSCs for PbSe, PbS, and CdSe/ZnS QDs are 0.26, 0.29, and 0.19 respectively. Thus, CdSe/ZnS suffer most drastically from increasing LSC size, which indicates that they suffer from self-absorption loss more significantly than the other two types of QDs. Although PbSe QD LSCs have the highest $\eta_{opt}$ by far, they display $\eta_{PCE}$ in between CdSe/ZnS QD LSCs and PbS QD LSCs due to the relatively low efficiency Ge solar cells coupled to the edges and low PL emission energies. Nevertheless, PbSe QD LSCs display the highest $F_{PCE}$ out of all three QD LSCs. Hence, they are the most effective QD fluorescent material for concentrating usable sunlight to the edges of the LSC waveguide and attached PV cells, which is the most important factor in an LSC design.
Chapter 6: LSC Design Optimization

6.1 – Employing Non-conventional PV Cells in LSC Systems

Conventional LSC designs in research often utilize high-efficiency c-Si or GaAs solar cells in an attempt to maximize the efficiency of the LSC system [22], [39], [43], [59]. Although these two types of solar cells are the benchmark for high-efficiency, single-junction solar cells due to their good I-V characteristics under solar-illumination, it is not necessarily sensible to use these types of solar cells in LSC systems. High-efficiency solar cells display excellent absorption and photo-conversion characteristics across the solar spectrum up to their respective cutoff wavelengths, and their band-gap and voltage is suited for optimum efficiency under solar-illumination, but that does not necessarily mean they provide the best performance under LSC edge illumination. The solar spectrum and the PL spectrum of common fluorescent materials are entirely dissimilar. Hence, the PV cells attached to the edges of an LSC should be optimized for highest efficiency under the PL spectrum of the embedded fluorescent material, rather than highest efficiency under solar-illumination.

Although LSC research is often driven by efficiency, the inherent purpose of an LSC is to reduce the cost of harvesting solar power relative to the cost of conventional PV cells. If LSCs cannot achieve this goal, any research directed toward improving efficiency is entirely ineffectual. Some types of extremely high-efficiency PV cells used in LSC studies, such as GaAs, are very cost prohibitive [60]. For LSCs to be cost competitive with other PV technologies, the materials and manufacturing cost of an LSC must be less than that of the “best value” PV cell currently produced; i.e. LSCs must be cost competitive with CdTe PV cells, which have a production cost of nearly $0.75/W with η_{pv} near 13% [46]. Furthermore, LSCs must be cost competitive with other BIPV technologies, especially those that function as translucent PV modules for window applications [61]. Since it is relatively uncommon to see LSCs with F_{PCE} greater than 20, and the highest performing LSC to date only has η_{PCE} of 7.1% [22], it may be more advantageous to utilize and reduce the cost of PV cells that already have low cost-per-watt values instead of trying to reduce the cost-per-watt of high-efficiency, high-cost PV cells to marketable levels. Thus, one solution is to utilize low cost PV cells with an EQE spectrum that matches well with the PL spectrum of a high η_{opt} fluorescent material/waveguide system to even further reduce the cost-per-watt value of harvesting sunlight. Since Red305 dye is currently the benchmark-performing, low cost fluorescent material for LSCs, it will be the focus for comparing the performance of PV cells in the following sections.

6.1.1 – Dye-Sensitized and Organic PV Cells in LSCs

Two types of PV technologies that may be able to function well in LSCs, which have not been previously studied in LSC designs, include dye-sensitized solar cells (DSSCs) [62], [63] and organic photovoltaic (OPV) cells [64]. Both types of PV cells are emerging PV technologies that use low cost materials and fabrication techniques to harvest solar power at reduced cost, albeit with lower power conversion efficiency than
conventional inorganic PV cells. Although the performance of DSSCs under concentrated sunlight is rarely studied, research has shown that the power conversion efficiency of DSSCs can improve to beyond 16% when exposed to solar irradiance concentrated by ~25x [65]. In comparison, the world record DSSC power conversion efficiency in non-concentrated sunlight is about 11% [66]. Thus, the use of DSSCs in LSCs is an intriguing prospect that may have been overlooked.

It is well known that OPV cells function more efficiently at smaller device dimensions [67], which is beneficial due to the fact that LSC designs require extremely small areas of PV cells to effectively concentrate sunlight. Organic PV cells tend to have relatively narrow absorption and quantum efficiency spectra due to the limited absorption range of organic materials. Though researchers often fabricate more complex, multi-junction OPV cells to expand the absorption range of OPV cells and improve efficiency [68], this may not be necessary or beneficial for LSC systems due to the relatively narrow PL emission spectra of fluorescent materials. Additionally, it may be advantageous to use several, specifically designed OPV cells with strong spectral responses in different color ranges that couple well to the emission spectra of different colored organic dyes for use in tandem LSCs. Though OPV performance tends to degrade in excessive sunlight concentration, studies have shown that OPV cells can be fabricated to develop maximum power conversion efficiency at around 4 to 12x solar concentration [69], which corresponds well with the concentration ratios often displayed by LSCs. Moreover, the degradation of OPV cells may be minimized by exposure LSC edge irradiance, rather than direct solar irradiance, due to the fact that harsh UV radiation will either be absorbed by the waveguide, down-converted by the fluorescent material, or simply transmit through the LSC system.

6.1.2 – Comparison of PV Cells for Optimal LSC Design

The PV cells simulated in this section include FhG-ISC GaAs [55], NaREC c-Si [40], ASP CdTe [57], Sony DSSC [57], and Konarka organic polymer Power Plastic® [57] PV cells. Due to the fact that FhG-ISC GaAs solar cells contributed to the highest efficiency LSC to date, as discussed in section 4.2.1, they are simulated as a reference to compare the other solar cells simulated in this section. According to a dissertation by Wilson, the cost of the simulated monocrystalline NaREC Si solar cells is nearly $4/W [40]. The simulated ASP CdTe PV cells have similar efficiency as currently produced First Solar CdTe PV cells which are presently produced for ~ $0.75/W. Since the EQE(λ) spectrum of First Solar CdTe cells could not be found, the ASP solar cells are assumed to be representative of First Solar PV cells, and therefore are assumed to cost $0.75/W. The Sony DSSC and Konarka OPV cell data are based on world record efficiency sub-module and cell measurements respectively, and are not representative of consumer-grade PV cells. Nevertheless, since the cost of these PV cells could not be found, they are assigned a cost of $1.00/W. Reference data for J_sc, V_oc, FF, η_{PV} and ($/W)_{PV} of the discussed PV cells under AM1.5 sunlight are shown in table 7.
Table 7: Reference data for various PV cells under AM1.5 solar illumination

<table>
<thead>
<tr>
<th>Company</th>
<th>PV Type</th>
<th>$\eta_{PV}$</th>
<th>$I_{SC}$ (mA/cm$^2$)</th>
<th>$V_{OC}$ (V)</th>
<th>FF</th>
<th>($$ / W_{PV}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>FhG-ISC</td>
<td>GaAs</td>
<td>23.2%</td>
<td>28.0</td>
<td>1.000</td>
<td>0.830</td>
<td>40.00</td>
</tr>
<tr>
<td>NaREC</td>
<td>c-Si</td>
<td>16.5%</td>
<td>33.6</td>
<td>0.620</td>
<td>0.790</td>
<td>4.00</td>
</tr>
<tr>
<td>ASP</td>
<td>CdTe</td>
<td>12.5%</td>
<td>21.2</td>
<td>0.838</td>
<td>0.705</td>
<td>0.75</td>
</tr>
<tr>
<td>Sony</td>
<td>DSSC</td>
<td>10.0%</td>
<td>19.4</td>
<td>0.719</td>
<td>0.714</td>
<td>&lt;1.00†</td>
</tr>
<tr>
<td>Konarka</td>
<td>OPV</td>
<td>8.3%</td>
<td>14.5</td>
<td>0.816</td>
<td>0.702</td>
<td>&lt;1.00†</td>
</tr>
</tbody>
</table>

† The cost-per-watt values of DSSC and OPV cells are approximate

It is important to note that reference values for $I_{SC}$ and thus $\eta_{PV}$ under AM1.5 illumination are ineffective quantities to analyze when attempting to understand how a PV cell will perform when attached to an LSC. On the other hand, $V_{OC}$ and $FF$ should be relatively similar for a PV cell regardless of whether it is illuminated directly by the solar spectrum or the PL spectrum of a fluorescent material, unless the concentration factor of the LSC is tremendously high. To characterize $I_{SC}$ under LSC edge illumination, the EQE(\(\lambda\)) curves of all the above solar cells need to be compared the PL spectrum of the fluorescent material embedded in the LSC waveguide as shown in figure 37.

**Figure 37:** Plot of EQE(\(\lambda\)) for GaAs [55], Si [40], CdTe [57], DSSC [57], and Organic [57] PV cells. The dotted line represents the photoluminescence spectrum of Red305 dye. The current generated in an LSC is dependent upon the degree of overlap between the EQE(\(\lambda\)) spectrum of the solar cells and the PL spectrum of the dye.

Since the PL spectrum will be the same regardless of the PV cell attached to the edge, the current produced in the PV cell will be directly proportional to EQE($\lambda_{PL}$). Thus, other than the fluorescent material and waveguide properties, there are only three primary factors that determine $\eta_{PCE}$ of an LSC: $V_{OC}$, FF, and EQE($\lambda_{PL}$) of the attached PV cells. Although the solar cell diode equations are likely to be inapplicable to DSSC and OPV cells, the superposition assumptions and solar cell diode equations used to
calculate power conversion efficiencies for inorganic PV cells are applied to OPV and DSSC cells in this analysis. Although $I_0$ is not directly applicable to DSSCs, a fictitious $I_0$ value is calculated from the reference $I_{SC}$ and $V_{OC}$ in AM1.5 solar illumination. The $I_{SC}$ developed in OPV cells tends to obey a power law relationship with incident irradiance, but can be approximated to be linear for solar concentrations less than 15 [69]. Additionally, the $V_{OC}$ developed in OPV cells tends to increase logarithmically with $I_{SC}$, which can be approximated using the solar cell diode equations assuming that overheating does not occur in the cell [69]. Using data from table 7 and figure 29, the relative EQE($\lambda_{PL}$) of various PV-LSC systems were predicted using the LSC Monte Carlo simulation software for a 50×50×5 mm$^3$ LSC embedded with 100μM of Red305 dye, as shown in table 8.

**Table 8:** Calculated EQE($\lambda_{PL}$) and relative $\eta_{PCE}$ of GaAs, Si, CdTe, DSSC, and Organic PV cells attached to a 50×50×5 mm$^3$ LSC with 100μM of Red305 dye.

<table>
<thead>
<tr>
<th>Fluorescent Material</th>
<th>PV</th>
<th>EQE($\lambda_{PL}$)</th>
<th>$\eta_{PCE}^{(GaAs)}$</th>
<th>$\eta_{PCE}^{(GaAs)}$</th>
<th>$F_{PCE}^{(GaAs)}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Red305</td>
<td>GaAs</td>
<td>0.95</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td></td>
<td>c-Si</td>
<td>0.95</td>
<td>0.59</td>
<td>0.83</td>
<td></td>
</tr>
<tr>
<td></td>
<td>CdTe</td>
<td>0.87</td>
<td>0.65</td>
<td>1.21</td>
<td></td>
</tr>
<tr>
<td></td>
<td>DSSC</td>
<td>0.68</td>
<td>0.44</td>
<td>1.02</td>
<td></td>
</tr>
<tr>
<td></td>
<td>OPV</td>
<td>0.73</td>
<td>0.53</td>
<td>1.48</td>
<td></td>
</tr>
</tbody>
</table>

The results from this calculation are quite fascinating. First and foremost, CdTe solar cells show great promise use in LSCs embedded with Red305 dye. Based on the data in table 7, the CdTe PV cells are expected to perform 65% as well as expensive, high-efficiency GaAs PV cells and 10% better than Si PV cells. Furthermore, CdTe PV cells are estimated to produce LSCs with $F_{PCE}$ 21% higher than GaAs PV cells and 46% higher than Si PV cells. Hence, not only do CdTe PV cells cost less per watt than GaAs and Si PV cells under solar illumination, they also have greater LSC-PV cost reduction factors when attached to the edge of an LSC. The poor short-wavelength response of CdTe PV cells, as shown in figure 35, encourages the use of down-shifting layers to convert high energy photons with a low probability of generating photocurrent to lower energy photons with a high probability of generating photocurrent. Also, as seen in figure 35, there is much potential to further increase photocurrent production in CdTe PV cells coupled to LSCs by utilizing a fluorescent material that absorbs throughout the entire visible spectrum and has a PL peak near ~800nm. Theoretically, it should be possible to fabricate quantum dots that provide this type of absorption/emission behavior, but the mediocre $\eta_{QY}$ and self-absorption loss exhibited by presently produced QDs is likely to hinder potential efficiencies. Based on the results of this analysis, the use of CdTe PV cells in LSCs should be investigated more deeply.

Another interesting fact of this analysis is that the Konarka Power Plastic® OPV cells, which are only 8.3% efficient under AM1.5 solar illumination, are anticipated to
perform 90% as well as Si PV cells that are 16.5% efficient under AM1.5 solar illumination. Also, in this configuration with organic PV cells, a PMMA waveguide, and Red305 dye, the LSC is an “all-organic” PV system. The estimated $F_{PCE}$ of Konarka OPV cells is higher than any of the other tested PV cells at 78% and 22% higher than Si PV cells and CdTe PV cells respectively. If the cost of the waveguide and fluorescent materials is ignored, the Konarka OPV cells simulated in this analysis have the highest LSC-PV cost reduction factor out of all the tested PV cells. However, since the cost per watt of the waveguide and fluorescent material are inversely proportional to $\eta_{PCE}$, and the cost of ultra-high efficiency OPV cells is relatively unknown, it cannot be said for certain whether CdTe or OPV cells are a more attractive candidate for LSC applications.

Dye-sensitized solar cells are anticipated to perform worse than all of the other PV cells, but their performance characteristics in concentrated sunlight are relatively unknown. Additionally, the use of diode equations is not physically applicable to DSSC cells. Thus, it will be much more fruitful to experimentally characterize the performance DSSCs in LSCs to obtain a better understanding of their performance under LSC edge illumination. Nevertheless, using the assumptions of this analysis, DSSCs in LSCs are expected to yield $\eta_{PCE}$ 75% as high as c-Si PV cells with 23% higher $F_{PCE}$. The efficiency analysis of this section provides evidence that the current conventions in place for selecting PV cells for LSCs must be re-evaluated.

6.2 – LSC Cost Optimization

To determine how LSC dimensions, fluorescent material concentration, PV type, and the use of a BSR in an LSC system affect cost, a cost-per-watt optimization analysis was performed for GaAs, Si, and CdTe and PV cells attached to a PMMA waveguide embedded with Red305 dye. Dye-sensitized and organic solar cells are not implemented in this cost study due to the fact that they tend not to obey diode superposition and their cost is somewhat unknown. Thus, they cannot be entirely accurately analyzed using the LSC Monte Carlo simulation software developed for this thesis. Though CdTe PV cells are not expected to obey diode superposition as well as p-n homojunction c-Si and GaAs PV cells, simulation results should be reasonable and the cost of these cells are well known. The material costs of LSC system components are listed in table 9.

Table 9: Unit cost of PMMA [40], Red305 dye [40], GaAs [60], c-Si PV cells [40], CdTe PV cells [46], and Aluminum mirror film used to calculate the cost of LSCs.

<table>
<thead>
<tr>
<th>Component</th>
<th>Type</th>
<th>$ / unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Waveguide</td>
<td>PMMA</td>
<td>$4800/m³</td>
</tr>
<tr>
<td>Fluor. Mat.</td>
<td>Red305</td>
<td>$16.00/g</td>
</tr>
<tr>
<td>PV Cell</td>
<td>GaAs</td>
<td>$9000/m²</td>
</tr>
<tr>
<td>PV Cell</td>
<td>c-Si</td>
<td>$660/m²</td>
</tr>
<tr>
<td>PV Cell</td>
<td>CdTe</td>
<td>$93.75/m²</td>
</tr>
<tr>
<td>BSR</td>
<td>Al</td>
<td>$3.00/m²</td>
</tr>
</tbody>
</table>
Since the cost of adding a BSR is likely to be less than the cost of the waveguide, it is expected that using a BSR will be advantageous with respect to efficiency and cost due to the fact that the thickness of the waveguide can be reduced by half without sacrificing efficiency since a BSR effectively doubles the solar absorption path length. If the waveguide thickness is reduced and efficiency is not sacrificed, the cost-per-watt of the waveguide, fluorescent material, and PV cells will all decrease directly proportionally to the thickness reduction of the waveguide. The relationship between the costs of each component relative to the cost of the entire LSC is complex, even more so due to the fact that the cost-per-watt of an LSC is not only dependent on the cost of the LSC itself, but also on $\eta_{PCE}$ and $P_{in}$.

It is important to note that all BSRs simulated in this study are simple specular mirrors due to limitations of the simulation, and the fluorescent material simulated in a single LSC layer is limited to a single dye. Since previous research suggests white scattering layers tend to perform even better than specular mirrors, and the addition of CRS040 dye to Red305 is capable of improving LSC edge emission by up to 10%, the efficiencies and costs obtained in this study can be further improved. On the other hand, due to the fact that host absorption, changes in fill factor with light concentration, and PV coupling losses are ignored, the results obtained in this study are likely to be within 10 to 20% error of actual, experimentally obtainable results. Parameter bounds for the optimization study must be emplaced to limit the possible number of LSC configurations and to realistically model LSCs within physical constraints. The parameter bounds used in the following optimization studies are shown in table 10.

| Table 10: Parameter bounds for the waveguide (PMMA) and fluorescent material (Red305) |
|-----------------|-----------------|-----------------|
| **Optimization Parameter** | **Lower Bound** | **Upper Bound** |
| Width           | 10mm            | 1000mm          |
| Length          | 10mm            | 1000mm          |
| Thickness       | 1mm             | 10mm            |
| Concentration   | 10μM            | 900μM           |

The lower bound for PMMA thickness of 1mm was emplaced due to the fact that fabricating an LSC with PV cells less than 1mm wide may pose manufacturing problems, and it is unknown how small PV cells can be manufactured while still maintaining similar efficiency and cost. The upper bound of width and length are emplaced due to the fact that host-absorption is ignored, and may pose loss problems at large LSC dimensions. The lower bound of width and length, and the upper bound of thickness of 10mm are only emplaced to limit extreme deviations from typical LSC size. The upper bound for Red305 concentration of 900μM was emplaced to avoid PL quenching effects [70]. On the following page, Table 11 and 12 show the efficiency and cost-per-watt results of a square LSC cost optimization study and rectangular LSC cost optimization study.
### Table 11: Cost optimization study of square LSCs utilizing PMMA waveguides and Red305 fluorescent material.

| Fluorescent Material | PV | BSR | $l_{LSC}$ (mm) | $W_{LSC}$ (mm) | $t_{LSC}$ (mm) | G | $c_x$ (µM) | $η_{opt}$ (%) | $η_{PCE}$ (%) | $F_{PCE}$ | $\frac{\$}{W_p}$ | $\frac{\$}{W_p}$ | $\frac{\$}{W_p}$ | $\frac{\$}{W_p}$ | $\frac{\$}{W_p}$ | $\frac{\$}{W_p}$ |
|----------------------|----|-----|---------------|---------------|----------------|---|------------|--------------|--------------|----------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|
| Red305               | GaAs | No   | 998          | 998           | 1              | 250 | 342       | 10.7         | 2.7          | 29        | 0.18          | 0.22           | 1.38           | -             | 1.77           |                |
|                      |     | Yes  | 965          | 965           | 1              | 241 | 263       | 14.2         | 3.6          | 39        | 0.13          | 0.13           | 1.06           | 0.08          | 1.41           |                |
|                      | c-Si    | No | 732          | 732           | 1              | 183 | 233       | 8.4          | 1.5          | 17        | 0.31          | 0.26           | 0.23           | -             | 0.81           |                |
|                      |     | Yes | 917          | 917           | 1              | 229 | 210       | 11.5         | 2.1          | 30        | 0.22          | 0.17           | 0.13           | 0.14          | 0.67           |                |
|                      | CdTe    | No | 328          | 328           | 1              | 82  | 349       | 17.7         | 2.4          | 16        | 0.20          | 0.25           | 0.05           | -             | 0.50           |                |
|                      |     | Yes | 235          | 235           | 1              | 59  | 246       | 22.3         | 3.0          | 14        | 0.16          | 0.14           | 0.05           | 0.10          | 0.45           |                |

### Table 12: Cost optimization study of rectangular LSCs utilizing PMMA waveguides and Red305 fluorescent material.

| Fluorescent Material | PV | BSR | $l_{LSC}$ (mm) | $W_{LSC}$ (mm) | $t_{LSC}$ (mm) | G | $c_x$ (µM) | $η_{opt}$ (%) | $η_{PCE}$ (%) | $F_{PCE}$ | $\frac{\$}{W_p}$ | $\frac{\$}{W_p}$ | $\frac{\$}{W_p}$ | $\frac{\$}{W_p}$ | $\frac{\$}{W_p}$ | $\frac{\$}{W_p}$ |
|----------------------|----|-----|---------------|---------------|----------------|---|------------|--------------|--------------|----------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|
| Red305               | GaAs | No   | 833          | 933           | 1              | 227 | 483       | 11.8         | 3.0          | 29        | 0.16          | 0.28           | 1.37           | -             | 1.81           |                |
|                      |     | Yes  | 879          | 1000          | 1              | 223 | 267       | 14.7         | 3.7          | 36        | 0.13          | 0.13           | 1.12           | 0.08          | 1.46           |                |
|                      | c-Si    | No | 620          | 725           | 1              | 167 | 330       | 9.7          | 1.8          | 18        | 0.27          | 0.32           | 0.22           | -             | 0.81           |                |
|                      |     | Yes | 775          | 900           | 1              | 208 | 213       | 11.7         | 2.2          | 28        | 0.22          | 0.17           | 0.14           | 0.14          | 0.67           |                |
|                      | CdTe    | No | 785          | 248           | 1              | 94  | 223       | 14.3         | 1.9          | 14        | 0.25          | 0.20           | 0.05           | -             | 0.50           |                |
|                      |     | Yes | 896          | 219           | 1              | 88  | 234       | 21.0         | 2.9          | 20        | 0.17          | 0.14           | 0.04           | 0.11          | 0.45           |                |
Interestingly, the lowest optimized cost-per-watt configuration for every simulated LSC was achieved at the lower bound of thickness of 1mm. This result intuitively makes sense due to the fact that absorption is an exponential process with respect to optical path length, but the cost of each component of an LSC, except for a BSR, scales linearly with thickness. Thus, the optimal thickness of an LSC with a BSR will be dependent upon the cost of the BSR relative to the cost of the waveguide. With the material prices assumed in this simulation, the cost of the waveguide will be equal to the cost of the BSR when the LSC thickness is nearly 620 microns, which is less than the lower bound of thickness. Thus, it is reasonable to expect that, unless the LSC thickness is near or less than ~0.6mm, it will always be advantageous to use a BSR from a cost perspective.

The absolute lowest cost-per-watt LSC configuration determined in this study was produced at $0.45/W_p from a square 235x235x1 mm³ LSC employing CdTe PV cells and a BSR with $\eta_{PCE}$ of 3.0%, which corresponds to a cost reduction factor of about 1.7 and efficiency reduction factor of about 4.2. Interestingly, the cost optimization study showed that both square and rectangular aspect ratios between $L_{LSC}$ and $W_{LSC}$ can produce LSCs with the nearly the same minimized cost. Multiple minimum cost configurations are beneficial due to the fact that certain applications and installations may be more conducive to using rectangular LSCs than square LSCs or vice versa. To determine the minimum theoretically attainable LSC cost that could be achieved with a better concentrator system, the loss mechanisms of the concentrator system must be analyzed. For the lowest cost LSC configuration determined in the study using CdTe PV cells, only 15.1% of solar photons were absorbed by the fluorescent material out of a possible 21.1% within the absorption range of Red305 and a possible 42.3% within the spectral response range of CdTe PV cells.

If a new fluorescent material is discovered that strongly absorbs to ~800nm instead of ~600nm as is the case for Red305, the potential number of solar photons that can be harvested would double. Assuming this is possible, and the amount of self-absorption loss was consistent, the power conversion efficiency of a CdTe PV LSC system could increase to nearly 6%, and the cost-per-watt would reduce to nearly $0.23/W_p or less. Self-absorption accounted for 29% relative loss in the CdTe PV LSC system. If researchers in the future discover a way to reduce or eliminate self-absorption loss, the efficiency of a CdTe PV LSC system would increase to nearly 4.25% or greater and the cost-per-watt of the LSC system would reduce to approximately $0.32/W_p or less due to the fact that the fluorescent material concentration and geometric gain could be increased without incurring more self-absorption loss. If both of these factors are combined together, and a new fluorescent material is discovered that absorbs strongly to nearly 780nm, emits shortly thereafter at ~800nm, and does not lose an appreciable amount of photons due to self-absorption loss, the power conversion efficiency of a CdTe PV LSC would be higher than 10%, and the estimated cost-per-watt of the LSC system would be less than $0.10/W_p. This data, in addition to the fact that installation costs could be offset due to building integration, suggests that LSCs are capable of becoming a significant commercial success if fluorescent materials are further improved, waveguiding techniques become more efficient, and self-absorption loss can be
mitigated. However, the pursuit of better material systems and waveguiding techniques have been sought after and studied for the last 40 years to no avail.

Although simulated LSCs employing GaAs and c-Si PV cells could not produce LSC systems with cost-per-watt values less than that of employing CdTe PV cells, the cost reduction factor of GaAs and c-Si LSC configurations are tremendous. The lowest cost of LSCs coupled to GaAs and c-Si PV cells were $1.41/W_p$ and $0.67/W_p$ with $\eta_{PCE}$ of 3.6% and 2.2%, cost reduction factors of 28.4 and 6.0, and efficiency reduction factors of 6.5 and 7.5 respectively. Given that the cost of polycrystalline Si (pc-Si) PV modules is expected to decrease to less than $1/W_p$, and the present performance of available pc-Si PV cells nearly matches that of the c-Si PV cell studied in this paper, the estimated, optimized cost-per-watt of an LSC employing 15.4% efficient pc-Si PV cells and a BSR is roughly $0.57/W$ with a $\eta_{PCE}$ of 2.52% at LSC dimensions of $275\times275\times1$ mm$^3$ with a Red305 concentration of 250μM. Thus, the estimated, optimized cost and efficiency of pc-Si PV cells used in LSCs is directly in between that of c-Si and CdTe. Also, the efficiency of the optimized pc-Si LSCs is higher than that of the optimized c-Si LSCs due to the fact that that geometric gain can be reduced to increase efficiency without incurring as much cost due to the lower base-price of the pc-Si PV cells.

Whether or not the LSC configurations determined in this study are useful and commercially viable is entirely dependent upon the required application of the LSC and the potential reduction of installation cost. Due to the thinness of the optimized LSC configurations, optimized LSCs are likely to be slightly flexible and light-weight. In fact, a PMMA waveguide with a thickness of 1mm, embedded fluorescent material, attached solar cells, and additional BSR should not weigh more than approximately 2kg/m$^2$, whereas conventional PV cells typically weigh more than 12kg/m$^2$ [71]. Given that the LSCs optimized in this section are so thin, they are not capable of being used to replace windows, but it may be possible to use thin LSCs with BSRs as window blinds for BIPV applications.
6.3 – Building Integrated LSC Design

Integrating solar harvesting devices into principal architecture is an important step for mainstream PV applications due to the fact that the costs of the PV cells can be offset by the costs that would typically be associated with the original building material. Luminescent solar concentrators can be used in building integrated photovoltaics in several different ways.

6.3.1 – Window LSC

Due to the fact that LSCs are translucent and use of large, planar glass and acrylic glass waveguides, LSCs can replace and enhance standard windows by offering power conversion capabilities, better thermal insulation, and added aesthetic value. Residential windows typically come in two different forms (single and double pane) [72], and two different thicknesses (single and double strength) [73]. Double pane windows, which are comprised of two window panes with an air gap between them, not only provide better heat and sound insulation than single pane windows, they also present an opportune avenue for tandem BIPV LSCs. Triple pane windows also exist, which could be used for triple-tandem LSC configurations, but they are relatively atypical in residential homes. Figure 38 shows an illustration of single, double, and triple pane windows.

![Figure 38: An illustration of single, double, and triple pane window glazing types [72]. (Image provided by Siding-1 Windows-1 Inc.)](image)

The difference between single and double strength glass windows is related to the thickness of the panes; single strength glass panes are typically 1/16 in. (~1.6mm) thick, and double strength glass panes are typically 1/8 in. (~3.2mm) thick. Due to the fact that LSC geometric gain increases and cost-per-watt reduces as thickness is reduced, single strength glass panes are likely to be better suited for LSC applications, but both can be utilized effectively.
To estimate the efficiency and cost of window-LSCs, optimization studies were performed for single and double pane windows with 1.6mm and 3.2mm panes. Double pane windows are designed to utilize tandem LSCs employing Lumogen® Red305 and Orange240 organic dyes; the absorption and emission spectra of Red305 and Orange240 are shown together in figure 39.

![Absorption spectrum and normalized emission spectrum of Lumogen® Red305 and Orange240](image)

**Figure 39:** Absorption spectrum and normalized emission spectrum Lumogen® Orange240 and Red305. The AM1.5 solar photon spectral irradiance is also shown to display spectral overlap.

Since Orange240 does not perform as well as Red305, but can better absorb higher energy photons in the solar spectrum, it is used as the embedded fluorescent material for the front LSC in double pane window-LSC configurations. Since a window is an essential component of the architecture, the cost of a window-LSC can be offset by the cost of the window itself. Thus, results will be reported for both the total material cost-per-watt of the window-LSC system ($C_{LSC}$) and for the cost-per-watt of the window-LSC system without factoring in the cost of waveguide ($C_{LSC}^*$). Due to the fact that rectangular and square LSCs tend to perform similarly with respect to cost and efficiency, the simulated window-LSCs will be square to simplify this analysis. Although a window-LSC cannot actively employ a permanent BSR, the efficiency of a window-LSC can be improved if white or mirrored window blinds are used to partially reflect light that is transmitted through the LSC. Nevertheless, BSRs are not factored into this analysis. Tables 13, 14, 15, and 16 show results for cost-optimized, simulated window-LSC systems for 1.6mm single pane, 3.2mm single pane, 1.6mm double pane, and 3.2mm double pane window systems respectively.
### Table 13: Cost optimization study of single pane, single strength (1.6mm) window LSCs.

| Fluorescent Material | PV | BSR | L_{LSC} (mm) | W_{LSC} (mm) | t_{LSC} (mm) | G | c_x (μM) | η_{opt} (%) | η_{PCE} (%) | F_{PCE} | $W_G$ (/W_p) | $F_M$ (/W_p) | $P_V$ (/W_p) | $LSC$ (/W_p) | $LSC^*$ (/W_p) |
|----------------------|----|-----|-------------|-------------|-------------|---|--------|------------|------------|---------|--------------|----------|-----------|-----------|-------------|--------------|
| Red305               | GaAs | No | 1000 | 1000 | 1.6 | 156 | 363 | 13.4 | 3.37 | 22.6 | 0.23 | 0.30 | 1.77 | 2.30 | 2.07 |
| c-Si                 | No | 948 | 948 | 1.6 | 148 | 227 | 10.5 | 1.95 | 17.5 | 0.40 | 0.32 | 0.23 | 0.95 | 0.55 |
| CdTe                | No | 470 | 470 | 1.6 | 73 | 193 | 16.9 | 2.29 | 13.5 | 0.34 | 0.23 | 0.06 | 0.62 | 0.29 |

### Table 14: Cost optimization study of single pane, double strength (3.2mm) window LSCs.

| Fluorescent Material | PV | BSR | L_{LSC} (mm) | W_{LSC} (mm) | t_{LSC} (mm) | G | c_x (μM) | η_{opt} (%) | η_{PCE} (%) | F_{PCE} | $W_G$ (/W_p) | $F_M$ (/W_p) | $P_V$ (/W_p) | $LSC$ (/W_p) | $LSC^*$ (/W_p) |
|----------------------|----|-----|-------------|-------------|-------------|---|--------|------------|------------|---------|--------------|----------|-----------|-----------|-------------|--------------|
| Red305               | GaAs | No | 1000 | 1000 | 3.2 | 78 | 227 | 17.0 | 4.23 | 14.2 | 0.36 | 0.36 | 2.82 | 3.55 | 3.18 |
| c-Si                 | No | 806 | 806 | 3.2 | 63 | 190 | 13.8 | 2.49 | 9.52 | 0.62 | 0.42 | 0.42 | 1.46 | 0.84 |
| CdTe                | No | 450 | 450 | 3.2 | 35 | 170 | 22.6 | 3.01 | 8.48 | 0.51 | 0.31 | 0.09 | 0.91 | 0.40 |
Table 15: Cost optimization study of double pane, single strength (1.6mm) window LSCs.

| Fluorescent Material | PV | BSR | L_{LSC} (mm) | W_{LSC} (mm) | t_{LSC} (mm) | G | c_x (μM) | η_{opt} (%) | η_{PCE} (%) | F_{PCE} | $W_G$ (W_p) | $F_M$ (W_p) | $P_V$ (W_p) | $LSC$ (W_p) | $LSC^*$ (W_p) |
|----------------------|----|-----|-------------|--------------|-------------|---|---------|-------------|-------------|--------|-------------|-------------|-------------|-------------|-------------|--------------|
| LSC 1: Orange240     | No | 1000| 1000        | 1.6          | 156         | 242| 18.3    | 4.56        | 15.3        | 0.34   | 0.38        | 2.61        | 3.32        | 2.99        |
|                      | No | 980 | 980         | 1.6          | 153         | 162| 14.4    | 2.61        | 12.1        | 0.59   | 0.32        | 0.33        | 1.24        | 0.65        |
| LSC 2: Red305        | No | 675 | 675         | 1.6          | 105         | 183| 22.5    | 3.04        | 12.8        | 0.51   | 0.30        | 0.06        | 0.87        | 0.36        |

Table 16: Cost optimization study of double pane, double strength (3.2mm) window LSCs.

<table>
<thead>
<tr>
<th>Fluorescent Material</th>
<th>PV</th>
<th>BSR</th>
<th>L_{LSC} (mm)</th>
<th>W_{LSC} (mm)</th>
<th>t_{LSC} (mm)</th>
<th>G</th>
<th>c_x (μM)</th>
<th>η_{opt} (%)</th>
<th>η_{PCE} (%)</th>
<th>F_{PCE}</th>
<th>$W_G$ (W_p)</th>
<th>$F_M$ (W_p)</th>
<th>$P_V$ (W_p)</th>
<th>$LSC$ (W_p)</th>
<th>$LSC^*$ (W_p)</th>
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</thead>
<tbody>
<tr>
<td>LSC 1: Orange240</td>
<td>No</td>
<td>1000</td>
<td>1000</td>
<td>3.2</td>
<td>78</td>
<td>159</td>
<td>22.5</td>
<td>5.53</td>
<td>9.28</td>
<td>0.56</td>
<td>0.37</td>
<td>4.31</td>
<td>5.24</td>
<td>4.68</td>
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</tr>
<tr>
<td></td>
<td>No</td>
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<td>990</td>
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<td>17.7</td>
<td>3.15</td>
<td>7.40</td>
<td>0.97</td>
<td>0.38</td>
<td>0.54</td>
<td>1.90</td>
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<tr>
<td>LSC 2: Red305</td>
<td>No</td>
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<td>807</td>
<td>3.2</td>
<td>63</td>
<td>128</td>
<td>26.2</td>
<td>3.50</td>
<td>8.80</td>
<td>0.88</td>
<td>0.31</td>
<td>0.09</td>
<td>1.28</td>
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<thead>
<tr>
<th>Fluorescent Material</th>
<th>PV</th>
<th>BSR</th>
<th>L_{LSC} (mm)</th>
<th>W_{LSC} (mm)</th>
<th>t_{LSC} (mm)</th>
<th>G</th>
<th>c_x (μM)</th>
<th>η_{opt} (%)</th>
<th>η_{PCE} (%)</th>
<th>F_{PCE}</th>
<th>$W_G$ (W_p)</th>
<th>$F_M$ (W_p)</th>
<th>$P_V$ (W_p)</th>
<th>$LSC$ (W_p)</th>
<th>$LSC^*$ (W_p)</th>
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<tbody>
<tr>
<td>LSC 1: Orange240</td>
<td>No</td>
<td>1000</td>
<td>1000</td>
<td>3.2</td>
<td>78</td>
<td>159</td>
<td>22.5</td>
<td>5.53</td>
<td>9.28</td>
<td>0.56</td>
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<td>LSC 2: Red305</td>
<td>No</td>
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<td>807</td>
<td>3.2</td>
<td>63</td>
<td>128</td>
<td>26.2</td>
<td>3.50</td>
<td>8.80</td>
<td>0.88</td>
<td>0.31</td>
<td>0.09</td>
<td>1.28</td>
<td>0.40</td>
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</table>
As stated previously, the cost of the window itself can be neglected because it is a required component of architecture. Thus, the costs discussed in this section will be restricted to the material cost of the fluorescent material(s) and attached PV cells only, disregarding the waveguide cost. For all window LSCs studied in both single and tandem configurations utilizing either c-Si or CdTe PV cells, the cost per watt peak of generating electrical power was less than $1/W. However, the efficiency of CdTe PV cell LSCs are 10% to 20% higher than c-Si PV cell LSCs, and the cost-per-watt-peak of CdTe PV LSCs is roughly half as much as c-Si PV cells. The additional materials cost of adding fluorescent material and PV cells to a window structure is roughly $0.30 to $0.40/W ($10 to $20/m²) for CdTe PV cells, $0.55 to $0.90/W ($15 to $30/m²) for c-Si PV cells, and $2.10 to $4.70/W ($70 to $260/m²) for GaAs PV cells. The modest power conversion efficiency improvement of 40 to 60% attained by using GaAs PV cells as opposed to CdTe PV cells comes at a staggering price difference of around 1000%. Thus, although GaAs PV cells can provide decent power conversion efficiency, especially if reflective window blinds were used to further enhance $\eta_{PCE}$, the cost premium is steep and the cost-per-watt-peak of generating power is higher than rooftop mounted PV cells.

Due to the fact that installing a window is much cheaper and easier than installing rooftop mounted PV cells, and a small inverter can be used to connect electronics directly to the window LSC system, relative installation cost will be negligible for a window-mounted LSC compared to conventional PV cells. Even so, the amount of power capable of being generated by an LSC is rather small unless many square meters of window area are available. In fact, nearly 30m² of window area would need to be available to generate 1kW of power in peak sunlight using CdTe PV LSCs. Thus, applications of window mounted LSCs will probably be limited to charging batteries and powering small appliances, rather than generating power for an entire home.

Though there is no doubt that window LSC systems can reduce the cost of harvesting solar power, for LSC systems to become truly useful and competitive with conventional PV cells, power conversion efficiencies need to be improved without increasing cost, whether it be by the discovery of new, highly absorbing and non-self-absorbing fluorescent dyes or the use of new waveguiding structures. Even so, window LSCs will probably be limited to niche applications, and are not likely to become mainstream power harvesting devices unless power conversion efficiencies can be significantly improved and/or the general population deems tinted windows to be aesthetically pleasing and desirable.
6.3.2 – Window Blind LSC

Instead of using LSCs in place of windows, it is also possible to use highly rectangular LSCs with BSRs in place of window blinds or shutters. Not only may this be advantageous with regard to installation, since windows will not need to be completely replaced, it may prove to be advantageous with respect to daily power conversion capability due to the fact that window blinds can use BSRs to reduce transmission loss and can rotate to track the sun throughout the day. Additionally, utilizing window-blind-LSCs offers the possibility of using double, triple, and even quadruple tandem LSC configurations if they are used in conjunction with single, double, and triple pane windows respectively. To mask the electrical connection between PV cells, electrical wiring can be interwoven with the blind-control cords, and an inverter or battery can be hidden inside the head-box of the blinds. Figure 40 shows an illustration of a red-emitting window-blind LSC system.

Figure 40: An illustration of a red-emitting window-blind LSC system.

To estimate the efficiency and cost of thin and long LSCs with BSRs that could be used as window-blinds, an optimization study was performed for window-blind-LSCs with $L_{LSC} \cdot W_{LSC} \geq 20$ employing Lumogen® Red305 dye as the fluorescent material. Additionally, PV cells were only simulated at a single long edge and mirrored film was simulated on the other three edges to enhance geometric gain. The length of each window-blind LSC is set at 2000mm, however, the length does not affect geometric gain since the PV cell is only attached to a single long edge. Thus, the results reported in this study will be reasonably valid for almost any LSC length that is much greater than its width. The thicknesses of the window-blind-LSCs simulated in this analysis are 0.5mm and 1mm for comparison. The results from the window-blind-LSC cost optimization study are shown in table 17.
Table 17: Cost optimization study of window-blind LSCs employing PV cells on a single long edge and mirrors on the other three edges. The length of each simulated LSC is 2000mm.

<table>
<thead>
<tr>
<th>PV</th>
<th>$W_{LSC}$ (mm)</th>
<th>$t_{LSC}$ (mm)</th>
<th>G</th>
<th>$c_x$ (μM)</th>
<th>$\eta_{opt}^e$ (%)</th>
<th>$\eta_{PCE}$ (%)</th>
<th>$F_{PCE}$</th>
<th>$\frac{$}{W_p}$</th>
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Based on the optimization results, window-blind LSCs perform very well compared to window-LSCs from a cost and efficiency perspective, especially for high efficiency PV cells such as GaAs. One of the primary advantages of using window-blind LSCs as opposed to window LSCs is due to the fact that window-blind-LSCs will not permanently tint and obstruct incident sunlight. Users will be able to open and close the blinds at will when they desire sunlight or shade respectively. Furthermore, the materials cost of window blind LSCs employing CdTe or Si PV cells is estimated to be in the same range as the cost of standard window blinds. In addition, window-blind LSC systems can be mass manufactured more easily than LSC windows because they do not have to fit to the exact dimensional specifications of a window frame. Moreover, diffuse BSRs can improve the power conversion efficiency of smaller LSC systems much better than specular BSRs [48]. Therefore, it is likely that real-world power conversion efficiencies of window-blind LSC systems using diffuse BSRs will be even better than the results reported in this analysis. All in all, the use of window-blind LSC technology should be investigated more deeply to determine real-world costs, efficiencies, and future market potential.
Chapter 7: Conclusions

7.1 – Accomplished work

The goals of this thesis were to develop accurate, robust, and user-friendly LSC Monte Carlo ray-tracing simulation software, analyze optical efficiency, power conversion efficiency, and cost of LSC systems, to propose and evaluate new ideas to improve the efficiency of LSCs, and to perform optimization studies to determine the viability of using LSCs to harvest solar power at reduced cost. To a reasonable extent, all of the anticipated goals have been realized.

7.1.1 – LSC Simulation

The accuracy of the simulation software for calculating the efficiency of LSC systems, as discussed in chapter 4, is typically within 10% error depending on the accuracy of the parameters and material properties used in the simulation. Due to the fact that error may stem from imperfect modeling of the incident solar spectrum, waveguide, fluorescent material, and PV cells, the total relative error of the simulation is quite good. The features of the LSC Monte Carlo simulation are fairly extensive as well. The simulation software is capable of characterizing the optical and electrical output of LSCs, as well as the impact of individual loss mechanisms and the cost-per-watt of each component of the system. Furthermore, the simulation software is capable of filtering data, performing sensitivity analyses, and performing optimization studies to determine the best design configurations. The dashboard user-interface allows users to easily adjust Monte Carlo simulation settings, select and tune LSC parameters, add ancillary features such as a BSR or tandem LSC, and view simplified simulation results pertaining to optical efficiencies, optical loss, power efficiencies, gain, and cost on a single page.

7.1.2 – Infrared Emitting LSCs

Modeling of infrared emitting PbSe QD LSCs in single and tandem LSC configurations were performed to determine the potential benefits of using an infrared harvesting layer to improve LSC power conversion efficiency, as discussed in chapter 5. Although PbSe QD LSCs are capable of effectively concentrating light, self-absorption loss and extreme photon down-conversion limits power conversion efficiencies to less than 2%, except at very small LSC dimensions. Based on simulation results, the addition of a tandem infrared harvesting LSC layer can only improve the efficiencies of stand-alone visible harvesting LSCs by about 10 to 20%. As the quality of infrared harvesting PV cells and infrared absorbing/emitting fluorescent materials improves, the use of an ancillary, infrared harvesting tandem LSC layer may prove to be beneficial for enhancing the power conversion efficiency of an LSC system. Also, the discovery of an efficient only-infrared absorbing and emitting fluorescent material would be useful for LSC designs due to the fact that LSCs could be made to look like ordinary transparent windows while harvesting incident solar power.
7.1.3 – Employing Non-Conventional PV cells in LSCs

Employing non-conventional PV cells in LSCs may be essential to the future success of LSC systems. Although PV cells used in LSC designs typically consist of high efficiency GaAs and Si solar cells, it is not necessary to use expensive PV cells that perform well throughout the entire solar spectrum. Rather, it is more important to select low cost PV cells that perform well specifically at the emission wavelengths of high efficiency fluorescent materials. CdTe PV cells are an excellent PV absorber candidate for LSC designs due to their low production cost and excellent spectral response at wavelengths within the emission spectrum of high efficiency fluorescent materials such as Lumogen® Red305. Organic PV cells may also be a viable candidate for use in LSC designs due to their low cost, high voltage output, and narrow spectral response that is couplable to the emission spectrum of fluorescent materials.

7.1.4 – Cost Optimization

Cost optimization studies were performed for LSCs employing PMMA waveguides, Red305 organic dye, and GaAs, c-Si, or CdTe PV cells as discussed in sections 6.2 and 6.3. The optimization parameters included length, width, thickness, and fluorescent material concentration. Due to the fact that reasonably high absorption efficiency can be attained within 1mm, and cost scales linearly with LSC thickness, the most cost effective LSC designs typically stem from the thinnest allowable LSC configurations, which were limited to 1mm in the study. Total cost-per-watt values as low as $0.45/Wp with power conversion efficiencies of 3.0% are achievable by using low-cost CdTe PV cells. Although cost-per-watt reduction factors of nearly 30 are achievable employing high-cost, high-efficiency GaAs PV cells, the total cost of the LSC is about $1.41/Wp, which is too high considering that the power conversion efficiency is only 3.6% at the dimensions and fluorescent material concentration for optimized cost.

7.1.5 – Building Integrated LSC Design

Building integrability is one of the often touted features of LSCs due to the fact that they are transparent to a portion of the solar spectrum and can be used as tinted windows. Given that the cost-per-watt of harvesting power reduces as LSCs become thinner, and the optical collection path length reduces as LSCs become less wide, it may also be advantageous to utilize LSCs as window-blinds or shutters rather than windows. Optimization studies were performed in section 6.3 to analyze the cost and efficiency of both window LSCs and window-blind LSCs. Both LSC configurations are certainly capable of reducing the cost-per-watt of harvesting solar power, but power conversion efficiencies tend to be less than 4%, which is far too low to be useful for generating power for an entire home. Although the power conversion efficiencies of LSCs are low, they are still more than capable of being used to charge batteries for mobile devices and power small appliances during the day. In the future, more research needs to be done to study the real-world cost, efficiency, and potential consumer demand for building-integrated LSC systems.
7.2 – Future Modeling Work

The robustness and accuracy of LSC Monte Carlo model can be improved by incorporating the following features into the simulation code.

7.2.1 – Diffuse BSR (White Scattering Layer)

Due to the fact that angle of incidence is assumed to be equal to the angle of reflection for every reflection event in the LSC Monte Carlo simulation, the trajectory and fate of a photon can be calculated in a single step. Although this method is computationally efficient, it restricts the model from being able to calculate a new trajectory for a photon after it interacts with an interface. To model a diffuse BSR, the model code will need to be changed to recalculate the trajectory of a photon after each interaction with any surface of the LSC. Since diffuse BSRs are known to improve LSC efficiency even more than specular BSRs, simulating LSCs with diffuse BSRs is important to obtain a more complete set of data for the efficiencies and costs of LSCs.

7.2.2 – Multiple Fluorescent Materials Embedded in a Single LSC

Sometimes it is advantageous to use multiple different dyes in a single LSC to achieve better absorption and emission properties than using a single dye. The LSC Monte Carlo simulation developed for this thesis is only capable of simulating one dye per LSC layer, but it is easily possible to incorporate two or more dyes into a single LSC layer without drastically altering the code. To model multiple dyes, competing absorption between multiple different fluorescent materials must be taken into account by generating separate absorption path lengths for each material as a photon is traversing through the LSC. The smallest absorption path length will correspond to the material that absorbs the photon first. Consequently, the emission properties of that material will be used for the following emission event, and the process will repeat until the photon is collected, transmitted, or lost due to NRR.

7.2.3 – Host-Absorption

Host-absorption, which occurs when the waveguide material itself absorbs photons as they traverse through an LSC, and is one of the major loss mechanisms associated with LSCs that is not modeled in the LSC Monte Carlo simulation. Host absorption is typically negligible for smaller LSC dimensions, but as the front surface area of an LSC increases, host-absorption becomes more prevalent. To model the effects of host-absorption, an additional absorption path length generated from the absorption spectrum of the waveguide material must be taken into account as a photon traverses through an LSC. If the randomly generated host-absorption path length is shorter than the collection path length and randomly generated self-absorption path length, the photon will be absorbed and lost due to host-absorption.
7.3 – Future Experimental Work

Almost all of the work done for this thesis was theoretical in nature. However, experimental studies need to be performed to properly evaluate the ideas proposed in this research. Also, experimental research is necessary to obtain new data for new types of fluorescent materials that may prove to be beneficial to an LSC design.

7.3.2 – Fabricating and Evaluating Infrared Harvesting LSCs

Though, in principle, an infrared emitting PbSe QD LSC was fabricated for this research, an infrared harvesting PV cell was not available to measure the electronic optical efficiency or power conversion efficiency of the concentrator system. Future work should focus on fabricating both visible and infrared harvesting LSCs and coupling them together to measure the power conversion efficiency gain obtainable by using a tandem visible/infrared harvesting LSC configuration.

7.3.3 – Fabricating and Evaluating Thin LSCs

Cost optimization studies in Chapter 6 showed that the best cost-per-watt LSC configurations were obtained when the LSC thickness was less than or equal to 1mm. Additionally, simulation studies showed that using CdTe PV cells instead of conventional Si PV cells may be advantageous for LSCs with respect to both efficiency and cost. Thus, experimental studies need to be performed to characterize the performance of small width (<1mm) CdTe PV cells and Si PV cells coupled to a thin (<1mm) LSC. Furthermore, the design of extremely small width PV cells needs to be further investigated to better understand the cost, efficiency, and feasibility of fabricating an LSC that is less than 1mm thick. Experimental studies should also be performed for high aspect ratio LSCs employing either specular or diffuse BSRs to evaluate the performance of window blind LSCs under both outdoor and indoor illumination.

7.4 – Final Remarks

Although LSCs are certainly capable of concentrating sunlight and reducing the cost of harvesting solar power, their power conversion efficiencies still need to be improved to compete with conventional PV cells. As has been the case since the incarnation of the LSC in the late 1970, the commercial viability of an LSC is dependent upon the development of new fluorescent materials with strong absorption throughout the entire visible spectrum, high fluorescence quantum yield, minimum absorption/emission spectrum overlap, and a life-span of at least 10 years. If dyes with reduced absorption/emission spectrum overlap cannot be developed, a greater focus will need to be placed on engineering waveguide structures that reduce the prevalence of self-absorption. In addition, researchers focusing on LSC development need to focus more strongly on the cost and light concentration capabilities of LSC devices rather than solely focusing on power conversion efficiency.
References


