Deciphering the uncertainties in life cycle energy and environmental analysis of organic photovoltaics†

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Organic photovoltaic (OPV) technologies are rapidly emerging as a viable alternative for traditional silicon and thin film technologies. OPVs are projected to be comparatively inexpensive and have a low energy payback time (EPBT) with lower levels of anthropogenic emissions during their lifetime. In this paper, we have analyzed the life cycle environmental impacts and EPBT of a scalable OPV module in the three cities Chicago, New York and San Francisco, for the current, near-term future and long-term future scenarios. Instead of using the deterministic or ‘single point estimate’ method, we employed a probabilistic approach by applying an uncertainty analysis to each of these scenarios using the Monte Carlo simulation method, and thereby quantifying the uncertainty and risk associated with each scenario. By comparing the proposed OPV technology with four typical silicon-based and thin-film photovoltaics in the aspects of EPBT and greenhouse gas (GHG) emissions, we demonstrate the great potential of OPVs in environmental sustainability. The probabilistic approach displayed a wide distribution for the EPBT and CO2 emission factor values, rather than squeezing around a single value. This demonstrated the insufficiency of deterministic analysis, which would give a false impression of certainty in the outcomes.

Introduction

Fossil fuels, a primary source of energy, are ravaging the environment and inducing climate changes due to their greenhouse gas (GHG) emissions. In contrast, the sun is the most abundant and clean source of energy available to us. Currently, the contribution of solar cells to global electricity production is only around 0.5%.1,2 It is expected that it will rapidly increase and will be a major contributor by the year 2060.3 However, they are currently too expensive to compete effectively with fossil fuels for electricity production (when hidden costs associated with fossil fuels are considered, this gap narrows considerably). Silicon-based (mono-Si, multi-Si, ribbon-Si) and thin-film (such as cadmium-telluride, gallium-arsenide, etc.) photovoltaic (PV) technologies account for the vast majority of the commercial market for PV technologies, representing the first and second generations of PV technologies, respectively.5,6 When it comes to recycling and disposal, silicon, cadmium, tellurium, gallium, arsenic, etc. are environmentally taxing.7 Thus the environmental sustainability of these technologies is questionable. The emerging

Broader context

Organic photovoltaics (OPVs) are among the most promising options for next-generation solar energy utilization, but for this technology to achieve broad market adoption a thorough understanding of the associated environmental impacts is needed—particularly with respect to current photovoltaic technologies. In this article, we apply a statistical approach to incorporate uncertainty associated with this type of analysis, and thereby capture not only important parameters such as energy payback time and greenhouse gas emission factors, but also a more realistic probabilistic picture of what values these parameters might take. From this analysis, we determine that, compared to traditional technologies such as silicon-based PVs, OPVs offer substantially shorter energy payback time and low carbon emissions even with current materials and processes. This advantage becomes truly striking when considering likely future technological advances in the field.

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technology of organic photovoltaics (OPV), referred to as a third generation PV technology,\textsuperscript{5,10} provides a solution to this problem. OPVs hold the promise of being an extremely economical technology,\textsuperscript{5,10} with low anthropogenic GHG emissions. OPVs have a much lower EPBT compared to mature commercialized PV technologies.\textsuperscript{1,11} OPVs make use of man-made materials and solution processing, instead of expensive and slow vapor phase deposition or vacuum-based deposition.\textsuperscript{12} (Studies have shown that vapor-based deposition should be avoided, due to the large EPBT, owing to the large process energies involved, and the low efficiencies of the resulting module.\textsuperscript{13}) This was made possible by the introduction of high purity conjugated polymers in the 1990’s.\textsuperscript{14,15} The main advantage is that the processing temperatures employed are much lower for OPVs as compared to inorganic counterparts. This feature allows for a wide choice of substrates, especially flexible polymer substrates, which can lead to lower cost. Additional advantages include their light weight and strong low-light performance. OPVs have not yet displaced conventional PV technologies because they have comparatively low efficiency relative to silicon-based PVs and thin film PVs.\textsuperscript{16}

When OPV technology started out, indium tin oxide (ITO) was widely used as an electrode, due to its conduction and optical properties.\textsuperscript{15,17} But indium is a rare and expensive element; this limits large-scale production.\textsuperscript{18,19} Thus, a number of attempts have been made to replace ITO with materials having similar properties, on a laboratory scale. Also, much work has already been done on the development of better materials and better designs for OPVs to increase their efficiency.\textsuperscript{20–38} The technology we refer to in this paper\textsuperscript{4} is one such example.

Life cycle analysis is a method that takes into account the environmental inputs and outputs of a process from its inception to its conclusion.\textsuperscript{39} It is necessary to ensure that new environmental issues are not created by the use of a technology and that technology decisions are based upon more complete knowledge of all the relevant parameters. A life cycle analysis has three aspects: energy, environmental and economic. Several groups have conducted life cycle analyses for all three generations of PV cells to calculate their energy payback time (EPBT) and GHG emissions.\textsuperscript{4,19,47} Espinosa et al. have demonstrated that replacing an existing technology with OPVs leads to very low GHG emissions and extremely short GHG-based pay back times.\textsuperscript{47} Also, a few papers have been written on the economic assessment of these technologies.\textsuperscript{5,19,48}

However, no work has been done on the application of an uncertainty analysis to the EPBT and environmental impacts of an OPV module, which is the focus of our paper. All previous LCA studies have been limited to a deterministic approach, but a probabilistic approach can allow us to understand the uncertainty and risks associated with a certain process or product. We consider the solar insolation, conversion efficiency, transport distance, performance ratio, system degradation rate and lifetime as the uncertain parameters, and analyze the effects of these uncertainties by using a Monte Carlo simulation. Uncertain conditions are introduced due to external factors like changes in weather and the operating conditions at the installation site, or internal factors like manufacturing defects, module design, etc. The data provided by the OPV module vendor is merely an approximation of its real world performance. Hence, the results obtained by using deterministic values of parameters could lead to inaccurate conclusions. An uncertainty analysis has a few critical advantages over a deterministic model.\textsuperscript{49} Due to the inherent uncertainty, the results obtained are probabilistic. They define the outcomes and also quantify the probability of their occurrence. Furthermore, conducting a sensitivity analysis also provides us with the extent to which the uncertain variables affect the EPBT and environmental impact of the technology. Capturing these uncertainties is critical to ascertaining the risks and benefits associated with commercializing the OPV technology. This will prove beneficial to investors by quantifying the variability of the results.

The roadmap of this paper is organized as follows. We first define the system boundary of our life cycle analysis, based on which we present the life cycle inventory (LCI) of the proposed OPV module, including the energy embedded in materials, direct process energy and energy for transport. Then we develop the model for quantifying the EPBT and GHG emissions, which are the two major metrics in the energy and environmental analysis. Later, after carefully identifying the proper assumptions and forecasts, we conduct the uncertainty analysis using Monte Carlo simulation for three geographically dispersed cities and three scenarios accounting for the current stage, near-term future and long-term future. In the end, we present detailed discussions for the results of the uncertainty analysis and make a comparison with four typical commercialized PV technologies to illustrate the great potential of OPVs in the aspects of energy and environmental sustainability.

**Materials and methods**

**System boundary**

The first step for performing a life cycle analysis is to determine the system boundary employed in the assessment. Depending on the interests and goals of different studies, the system boundary can be defined in various ways. The most common options involve “cradle to grave”, “cradle to gate”, “gate to grave” and “gate to gate”.\textsuperscript{49} In this work, we adopt the cradle-to-gate system boundary considering all processes from the raw material extraction through the production phase, and the transport of finished products from manufacturing sites to the gate of vendors. As illustrated in Fig. 1, the use phase and disposal phase of the product are not incorporated in the system boundary, which indicates a partial life cycle of the product. The transport phase of raw materials is omitted in this study, as we assume that the raw materials can be obtained locally. This assumption is generally justified for OPV processes as chemical synthesis can be carried out largely irrespective of geography.

![Fig. 1 System boundary of the life cycle analysis.](image)
Life cycle inventory (LCI)

LCI refers to a list where all the materials and energy supplies and emissions throughout a product’s life cycle are gathered. According to the system boundary depicted in the previous section, the LCI can be divided into three categories: energy embedded in materials, direct process energy and energy for transport, which will be addressed respectively in later sections.

In this work, our analysis will be focusing on a particular kind of OPV using a promising manufacturing technology reported at Risø DTU, which is denoted as “Process H” in the original paper. Compared to other manufacturing routes, although the module efficiency may not be as high as other alternatives, this process leads to significant reductions in energy costs and avoids the use of rare elements having limited supply. These attributes would greatly facilitate up-scaling. Since the specific product produced by this process has not been commercialized yet, the data used for the analysis are obtained from pilot-scale experiments. Future processes could incorporate higher performance materials and more efficient processing technologies, which could increase device lifetime and/or power conversion efficiency.

The functional unit (FU) is defined as 1 m² OPV modules in this study. All the inputs and outputs in the LCI are measured in terms of this functional unit. The energy budgets embodied in the module were converted to equivalent primary energy (EPE) units, where we consider the average electrical conversion efficiency as 35% and the average thermal conversion efficiency as 85%.

Energy embedded in materials

Since the technical details of the manufacturing technology is not the interest of this article, we only present a summary of the material inventory and cumulative energy demand (CED) for the raw materials production. Further information can be found in the ESI† or one can refer to the original paper by Espinosa et al.1

As shown in Table 1, the total energy required in producing raw materials for 1 m² OPV modules is 22.91 MJₑₚₑₑ, of which the major contributions come from the PET substrate, PEDOT:PSS, adhesive and PET encapsulation. Efforts on reducing the use of PET and adhesive are ongoing. Also, novel materials replacing PEDOT:PSS have been reported for the hole transport layer (HTL). Espinosa et al. have successfully explored the use of hydrated vanadium(v) oxide in the large scale and R2R fabrication of inverted PEDOT-free polymer solar cells. However, since the data of these cutting edge technologies are beyond reach, we will use the data reported in the original paper by Espinosa et al. for our analysis.

Direct process energy

The manufacturing of this kind of OPV modules involves six processing stages: front electrode processing, electron transport layer (ETL) deposition, active layer deposition, PEDOT:PSS deposition, back electrode deposition and lamination. The energy consumption of these processes is dominated by electricity input. Hence, in order to facilitate comparison and calculation, the electrical energy consumption is converted into EPE by dividing by the electrical conversion efficiency as given in Table 2. The total energy cost in the production of 1 m² OPV modules is measured as 21.91 MJₑₑₑ.

Energy for transport

In this study, we consider three geographically dispersed locations (Chicago, IL, New York City, NY and San Francisco, CA) as potential markets in the US for this kind of polymer solar cells due to their large populations and significant energy consumptions. We assume the manufacturing site will be installed near Phoenix, AZ, which has a vast open area for building plants and abundant human resources.

The finished products will be transported from Phoenix to the above three cities by truck. The energy intensity of road transport used in this study is estimated as 0.0034 MJₑₑₑ kg⁻¹ km⁻¹, according to the International Energy Agency (IEA) Database. The weight of the polymer solar cell modules (0.221 kg m⁻²) can be obtained by summing up the units of raw materials listed in the second column in Table 1. The energy cost for transporting

Table 2 | Direct process energy of 1 m² of OPV modules (W hₑₑₑ)¹

<table>
<thead>
<tr>
<th>Process</th>
<th>Energy (W hₑₑₑ)</th>
</tr>
</thead>
<tbody>
<tr>
<td>S1 Front electrode processing</td>
<td>10.93</td>
</tr>
<tr>
<td>Electrode coating</td>
<td>10.93</td>
</tr>
<tr>
<td>Drying</td>
<td>245.90</td>
</tr>
<tr>
<td>S2 ET layer deposition</td>
<td>81.97</td>
</tr>
<tr>
<td>ZnO slot die coating</td>
<td>81.97</td>
</tr>
<tr>
<td>Drying</td>
<td>368.85</td>
</tr>
<tr>
<td>S3 Active layer deposition</td>
<td>5.57</td>
</tr>
<tr>
<td>P3H6:PCBM ink preparation</td>
<td>5.57</td>
</tr>
<tr>
<td>P3H6:PCBM slot die coating</td>
<td>40.98</td>
</tr>
<tr>
<td>Drying</td>
<td>368.85</td>
</tr>
<tr>
<td>S4 PEDOT:PSS deposition</td>
<td>1.31</td>
</tr>
<tr>
<td>PEDOT:PSS ink preparation</td>
<td>1.31</td>
</tr>
<tr>
<td>PEDOT:PSS slot die coating</td>
<td>74.52</td>
</tr>
<tr>
<td>Drying</td>
<td>670.64</td>
</tr>
<tr>
<td>S5 Back electrode deposition</td>
<td>10.93</td>
</tr>
<tr>
<td>Slot die coating</td>
<td>10.93</td>
</tr>
<tr>
<td>Drying</td>
<td>245.90</td>
</tr>
<tr>
<td>S6 Lamination</td>
<td>4.10</td>
</tr>
<tr>
<td>Encapsulation by R2R lamination</td>
<td>4.10</td>
</tr>
<tr>
<td>Subtotal (W hₑₑₑ)</td>
<td>2130.45</td>
</tr>
<tr>
<td>Subtotal (MJₑₑₑ)</td>
<td>21.91</td>
</tr>
</tbody>
</table>

¹ R2R: roll-to-roll.
OPV modules will be calculated as the product of the energy intensity of road transport, weight of modules and transport distance.

**Energy payback time (EPBT)**

EPBT is one of the most frequently used metrics for PV system sustainability analysis. EPBT is defined as the period required for an energy system to generate the same amount of energy that was consumed during its life cycle.\(^{39}\) According to the system boundary defined in our study, the EPBT can be represented as,

\[
\text{EPBT} = \frac{\text{EM} + \text{EP} + \text{ET}}{\text{EG}}
\]

(1)

where EM is the energy embedded in materials; EP is the direct process energy; ET is the energy for transport and EG is the annual electricity generation of the OPV module in terms of primary energy. The first three terms were obtained following the previous discussion, while the calculation of EG is given by,

\[
\text{EG} = \frac{I \times p \times \text{eff} \times a}{0.35}
\]

(2)

where \(I\) is the annual average insolation predicted from historical data. \(p\) is the performance ratio, which is a commonly used parameter for a complete PV system (inverter, wiring, contamination in the modules, etc.) that takes into account losses. A 20% loss is often assumed in operating PV systems, thus suggesting a performance ratio of 80%. \(\text{eff}\) stands for the power conversion efficiency on the active area, which is the primary indicator of the energy generation capability of solar cells. \(a\) represents the percentage active area on the module. 0.35 is the electrical conversion efficiency for converting the unit into EPE.

**Greenhouse gas (GHG) emissions**

GHG emissions over a product’s life cycle indicate its environmental impact on the global climate. This metric is especially important as global warming issues arouse increasing attention. As a standard measurement, CO\(_2\) equivalency is generally used, which is a quantity that describes, for a given mixture and amount of GHG, the amount of CO\(_2\) that would have the same global warming potential (GWP), when measured over a specified timescale (generally, 100 years), where GWP is a relative measure of how much heat a GHG traps in the atmosphere. The equivalent CO\(_2\) emissions can be obtained by multiplying all energy and material inputs with their corresponding CO\(_2\) emission factors.\(^{40}\) Since most of the energy inputs to the module are electricity inputs, for simplicity, we convert the EPE to electricity and calculate the CO\(_2\) emissions related to 1 m\(^2\) of OPV modules by multiplying the average electricity mix. This parameter is highly dependent on the fuel mix of the considered utility system.\(^{41}\) For the southwest US where our manufacturing site is located, this value is 913.09 g eq. CO\(_2\) per kW h\(_{el}\).\(^{57}\)

Based on the above discussion, the embodied CO\(_2\) emission is given by,

\[
\text{EC} = (\text{EM} + \text{EP} + \text{ET}) \times 0.35 \times \text{elmix}
\]

(3)

where EC is the embodied CO\(_2\) in the module; elmix is the average electricity mix.

The above calculation shows the total amount of CO\(_2\) emissions involved in the partial life cycle of the OPV modules, including the raw materials extraction, production phase and the transport of finished solar cells. However, one would perhaps be more interested in the “CO\(_2\) price” related to each kW h of generated electricity, which is called the CO\(_2\) emission factor. This parameter is calculated as the total embodied CO\(_2\) emissions of the module divided by the total generated electricity over the module’s lifetime. As this type of OPV module is projected to last for about 15 years,\(^{39}\) the system degradation rate should also be taken into consideration. (Note that current lifetimes of commercial OPV modules are typically shorter than this value.) The rate at which solar cell performance degrades may be affected by various factors, such as the quality of manufacturing, power production level, and local weather/climate.

Since the system degradation rate has a cumulative effect on the performance of OPV modules, the total generated electricity can be treated as the summation of the elements in a geometric progression (demonstrated in the ESI†). Hence, the CO\(_2\) emission factor is calculated by,

\[
\text{EF} = \frac{\text{EC} \times \text{sd}r}{\text{EG} \times [1 - (1 - \text{sd}r)^n]}
\]

(4)

where EF is the CO\(_2\) emission factor; sd\(r\) is the annual system degradation rate and \(n\) is the lifetime of the module.

**Uncertainty analysis**

So far, we have developed a model for calculating the EPBT and CO\(_2\) emission factor, which are two major indicators of life cycle analysis. We have also explored the static relationship between various parameters, among which some will be fixed once a processing technology is selected and a manufacturing site is settled, e.g., the amount of raw materials required per functional unit, the percentage active area and the average electricity mix. However, some parameters have inherent uncertainties. For instance, one will never know exactly how long a polymer solar cell is going to last. Though an accurate prediction of the values of these parameters is impossible, we can assume reasonable probability distributions for these parameters based on our insights on their properties and the analysis of historical data.

We apply simulation methods to investigate how the uncertainties in these varying parameters influence the major sustainability indicators (EPBT and CO\(_2\) emission factor), thus presenting a dynamic perspective of the energy consumption and environmental impact of the OPVs. We employ the spreadsheet-based application suite, Oracle Crystal Ball,\(^{59}\) as our research tool, using the Monte Carlo simulation method to perform the uncertainty analysis. During the Monte Carlo simulation, values of varying parameters are sampled randomly from the input probability distribution. Each set of samples is called an iteration, and the resulting outputs are recorded. By conducting a sufficient number of iterations, a “pool” of outputs resulted from thousands or millions of sets of samples will be gathered for analysis.

Different from the deterministic, or “single-point estimate” method that is widely used in the literature for life cycle analysis, the results from Monte Carlo simulations tell not only what would happen, but also how likely it is to happen by presenting
Assumptions and forecasts

In Oracle Crystal Ball, the uncertain input is called an “assumption”, and the resulting output is called a “forecast”. We specify in our model six assumptions and two forecasts, as summarized in Table 3. The OPV manufacturing data here is from a pilot-scale study, which can reasonably be compared to that of a commercial setup. According to the available OPV technologies, three scenarios different in the power conversion efficiency of the active area and percentage active area are considered, accounting for the current stage, near-term future (1–2 years) and long-term future (~5 years), respectively. Note that the percentage active area is not an assumption in our analysis but rather a fixed parameter in each scenario. The reason for considering the percentage active area in the scenario is that one can anticipate the improvement in manufacturing technologies and module designs that would take full advantage of the processed area in the future.

Though other parameters may also be affected by physical location, in this study we assume only the road transport distance and annual insolation vary for different cities. The road transport distance is accounted as an assumption, because it depends greatly on the road condition, weather/climate and sometimes change of routes may be required. The mean value of the transport distance is obtained from Google Maps. The standard deviation is roughly estimated by the authors and we assume a larger distance usually results in larger variance. The probability distributions of annual insolation in Chicago, New York City (NYC) and San Francisco (SF) are predicted employing the time series method based on the historical data from 1961 to 1990 provided by the National Renewable Energy Laboratory. In this study, we assume the panels are installed as a flat-plate collector facing south at fixed tilt equal to the latitude.

A prediction into 20 years in the future is performed using the “predictor” tool in Oracle Crystal Ball. A mean value and a standard deviation are obtained, which will then serve as the parameters for the normal distribution. In this analysis, we assume the system degradation rate follows a gamma distribution, which accounts for a small number of unusually poor performers as is often observed in practice. For simplicity, we treat the system degradation rate as a single value in CO2 emission factor calculations in spite of the fact that an OPV module may degrade at different rates along its lifetime. The parameters for this gamma distribution are selected to bear qualitative resemblance to real-world systems. The assumption of a lifetime of 15 years is as projected by the European Photovoltaic Technology Platform for OPVs for the year 2013. The values for the performance ratio and the conversion efficiency are derived from existing literature. The values for the standard deviations for the performance ratio, conversion efficiency and lifetime have been estimated by the authors. The performance ratio and lifetime can change with location, but for this study, we have made a simplification, assuming that these parameters do not depend on external factors. Note that the objective of this work is the development of a generic model for uncertainty analysis. The model can adapt as new data emerge.

Results and discussions

Uncertainty analysis of EPBT

Using the model proposed in the previous section, we performed the simulation for 1 million trials (iterations). The probability distributions of the EPBT of each scenario and each city are presented in Fig. 2 as a matrix. The values of the mean and standard derivation are also given in the graph. We can see that the EPBT displays a wide distribution, rather than squeezing around a single value. This further demonstrates the insufficiency of deterministic analysis, which would give a false impression of

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Scenario 1</th>
<th>Scenario 2</th>
<th>Scenario 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Performance ratio</td>
<td>Normal distribution</td>
<td>Normal distribution</td>
<td>Normal distribution</td>
</tr>
<tr>
<td>Mean</td>
<td>0.8</td>
<td>0.1</td>
<td>0.1</td>
</tr>
<tr>
<td>Std. dev.</td>
<td>0.03</td>
<td>0.05</td>
<td>0.08</td>
</tr>
<tr>
<td>Conversion efficiency</td>
<td>Normal distribution</td>
<td>Normal distribution</td>
<td>Normal distribution</td>
</tr>
<tr>
<td>Mean</td>
<td>1598.19</td>
<td>60.26</td>
<td>1598.19</td>
</tr>
<tr>
<td>Std. dev.</td>
<td>6162.78</td>
<td>50.84</td>
<td></td>
</tr>
<tr>
<td>Insolation in Chicago (kW h m^{-2} \text{year}^{-1})</td>
<td>Normal distribution</td>
<td>Normal distribution</td>
<td>Normal distribution</td>
</tr>
<tr>
<td>Mean</td>
<td>1956.51</td>
<td>58.87</td>
<td>1956.51</td>
</tr>
<tr>
<td>Std. dev.</td>
<td>2875</td>
<td>250</td>
<td>2875</td>
</tr>
<tr>
<td>Road distance to Chicago (km)</td>
<td>Normal distribution</td>
<td>Normal distribution</td>
<td>Normal distribution</td>
</tr>
<tr>
<td>Mean</td>
<td>4100</td>
<td>300</td>
<td>4100</td>
</tr>
<tr>
<td>Std. dev.</td>
<td>1210</td>
<td>200</td>
<td>1210</td>
</tr>
<tr>
<td>Lifetime (year)</td>
<td>Normal distribution</td>
<td>Normal distribution</td>
<td>Normal distribution</td>
</tr>
<tr>
<td>Mean</td>
<td>15</td>
<td>0.5</td>
<td>15</td>
</tr>
<tr>
<td>Std. dev.</td>
<td>0.006</td>
<td>2</td>
<td>0.006</td>
</tr>
</tbody>
</table>

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certainty in the outcomes. Overall, the peaks stand for the most likely EPBTs. It is interesting that the peak maxima occur not at the mean but slightly on the left of it. This is due to asymmetry of the probability distribution profiles, rising relatively faster on the left side while leaving a long tail on the right side. The asymmetry reflects the nonlinear relationship between the inputs and outputs.

In a horizontal comparison, the performance of polymer solar cells located in the same city but under different scenarios is presented. As an example, for the OPV modules installed in Chicago, the mean of the EPBT decreases from Scenario 1 (101.35 days) to Scenario 3 (19.59 days). This indicates that the increase in conversion efficiency and percentage active area would largely reduce the EPBT. We can also observe a remarkable decrease in the standard deviation from Scenario 1 (23.48 days) to Scenario 3 (2.96 days). The trend suggests that the improvement in conversion efficiency and percentage active area will also increase the certainty of EPBT. This sort of information is of tremendous potential value to investors who want to ascertain the risk associated with the commercialization of this technology.

In a vertical comparison, the performance of the OPVs located in different cities but under the same scenario is investigated. As an example, for Scenario 2, it is no surprise that the modules installed in San Francisco have the shortest EPBT (31.80 days) while Chicago exhibits the longest (40.03 days), because San Francisco has the highest annual insolation and Chicago the lowest of the locations analyzed here. Note that the road transport distance also contributes to the EPBT. But as will be discussed later, the effect of distance can be neglected.

We also performed sensitivity analysis to examine how the variance in input parameters would influence the EPBT. For illustration, here we only present the results for OPV modules installed in Chicago under Scenario 2, representing the technology in the near-term future. Since the EPBT of polymer solar cells is much shorter than a year, we exclude the effects of lifetime (which is much longer than the EPBT) and system degradation rate (which is usually measured on a yearly basis). Hence, only four assumptions are considered in the analysis (performance ratio, conversion efficiency, insolation and transport distance). As shown in Fig. 3 the power conversion efficiency and the performance ratio have a dominant effect on the uncertainty of the EPBT. The performance ratio accounts for 58.4% of the variance in forecast values and is the most important assumption in the model, while the conversion efficiency accounts for 36.6%. The negative sign indicates a negative correlation between the input and output. For instance, increase in the performance ratio would result in shorter EPBT. Variances in the insolation contribute to 5% of the uncertainty in EPBT, which is small but not negligible. However, the transport distance accounts for merely 0.1%. This is due to the fact that the energy consumption during the transport phase only accounts for a small portion of the total energy cost. We can draw a conclusion from the sensitivity analysis that if one wants to reduce the uncertainty in the EPBT, control of the variances in power conversion efficiency and the performance ratio would be the direction for further investigation. The latter can usually be achieved by better module design, standard production and quality control, etc. while the former will benefit from development of new materials and light management strategies.

Tornado charts (Fig. 4) and spider charts (Fig. 5) offer us another view of the sensitivity analysis. The tornado chart illustrates the swing between the maximum and minimum forecast values as each variable swings within a pre-specified range.
The variable that causes the largest swing is displayed at the top and the variable that causes the smallest swing at the bottom. This corresponds to our previous conclusion. A spider chart illustrates the differences between the minimum and the maximum forecast values by graphing a curve through all the values tested. Steeper slopes indicate larger influences on forecast values while positive–negative slopes suggest positive–negative correlations. In Fig. 5, we present results on 10 testing points. The performance ratio and the conversion efficiency display steep negative slopes, but the curve for the transport distance is almost a horizontal line. Also, it is worth mentioning that the curves in Fig. 5 are nonlinear, which demonstrates the nonlinearity of the relationship between assumptions and forecasts from another perspective.

Analysis of GHG emissions under uncertainty

Similar to the uncertainty analysis of the EPBT, the probability distributions of the CO₂ emissions factor for Chicago, NYC, and San Francisco under three scenarios are presented in Fig. 6. We can draw the similar conclusions for the EPBT from the horizontal and vertical comparisons. The improvements in conversion efficiency and percentage active area would increase the total generated electricity over a module’s lifetime thus lowering the “CO₂ price”. A higher insolation would always be beneficial to the reduction of GHG emissions. Notice that all 6 uncertain parameters (solar insolation, conversion efficiency, transport distance, performance ratio, system degradation rate and lifetime) are considered this time. Again, we performed sensitivity analysis for Chicago under Scenario 2 as presented in Fig. 7; we observe that the conversion efficiency and the performance ratio are still the most important assumptions affecting the variances in the CO₂ emission factor, which account for 51.4% and 32.3%, respectively. But the effect of system degradation rate is also significant, which contributes to 9% of the uncertainty in the CO₂ emission factor. The system degradation rate displays a positive correlation to the CO₂ emission factor. The reason is that an increase in the system degradation rate would result in a decrease...
in total generated electricity over a module’s lifetime, thus causing a higher “CO₂ price” per functional unit. As supplementary analysis, the tornado chart and the spider chart of the CO₂ emissions factor for Chicago under Scenario 2 are presented in Fig. 8 and Fig. 9.

Consistent with the previous discussion, the performance ratio, conversion efficiency and system degradation rate rank the first three in their influence on the CO₂ emissions factor, and the effects of transport distance can be neglected. Once again, the nonlinear relationships between inputs and the outcomes are illustrated in the spider chart.

Comparison with commercialized PVs

The previous sections provide a thorough energy and environmental analysis for the proposed OPV technology. However, in order to evaluate investment value of OPV projects, comparisons with existing solar cells are required. The comparison of future OPV technology with current commercialized PV technologies might appear biased, but considering that OPV technology is still in its infancy, the room for improvement of OPVs is likely large compared to other PVs. In this section, we will present comparisons in EPBT and equivalent CO₂ emissions factor with commercialized silicon-based and thin-film PVs. The data for silicon-based PVs are estimated with Southern European insolation 1700 kW h m⁻² per year, performance ratio of 0.75, and a lifetime of 30 years (of which the annual insolation is higher than that in Chicago, ~1600 kW h m⁻² per year and the performance ratio is lower than that used in our analysis, 0.8, thus forming a tradeoff in EPBT and making the results comparable). The data for CdTe PVs are obtained under the same solar insolation as in our analysis, performance ratio of 0.83, and a lifetime of 30 years (of which the performance ratio is inconsiderably higher, thus making the comparison slightly more favorable to CdTd PVs).

Note that the balance of system is not included in the analysis. For the proposed OPV, we present the results for Chicago under three scenarios representing the current stage, near-term future and long-term future.

Fig. 10 shows a remarkable advantage of the OPV technology over other PVs in EPBT. Even at the current stage with a relatively lower conversion efficiency of 3%,⁴ the EPBT of OPVs is shorter than half that of CdTe PVs, which represent the best performance among the four commercialized PVs. This is because the embodied energy of OPVs is much lower than its silicon-based and thin-film counterparts, mostly due to the low-temperature processing and flexible choice in plastic substrates. Looking into Scenario 2 (EPBT of 40 days) and Scenario 3 (EPBT of 20 days) for the OPV technology, one could even aggressively anticipate the improvement in processing technologies and the development of novel materials to result in a one-day energy payback in future decades.

Fig. 11 demonstrates the comparison between the CO₂ emission factors. Again, CdTe PVs display the best performance among the four commercialized PVs. At the current stage, the GHG emissions of the proposed OPV technology is slightly higher than that of CdTe PVs. However, it is worth mentioning that the emissions from CdTe PVs are mostly heavy metals, rather than GHGs, due to the treatment and use of cadmium and tellurium. Since the development of OPVs is still at its infancy, significant reduction in GHG emissions is likely to be achieved in the foreseeable future as suggested by Scenario 2 and Scenario 3.
As per our assumptions, the EPBT is not limited by the lifetime of the cell. Thus, comparing technologies with a different lifetime to OPVs will clearly show the advantage of OPVs in that respect. The CO₂ emission factor is dependent on the lifetime of the cell. Thus, comparing OPVs with other technologies having longer lifetimes will not show the advantages of OPVs as clearly. Efforts in prolonging the lifetime of OPVs will be highly beneficial in this regard.

**Conclusions**

OPV technology representing the third generation of PVs is predicted to be a promising solution in addressing the future 1 GW daily growth in energy demand at a global level. Unlike its silicon-based and thin film counterparts, OPVs have not been commercialized on a large scale yet. To confirm the environmental sustainability of OPV technology, we perform a cradle-to-gate life cycle analysis based on a recent OPV processing technology reported at Risø DTU. Instead of using the deterministic analysis method, we adopt Monte Carlo simulation to explore not only the static aspects of the energy and environmental impact, but more importantly the inherent uncertainty in OPV systems. In this work, we conduct life cycle analysis for three potential markets geographically dispersed in the US, as well as three scenarios accounting for the current stage, near-term future and long-term future. By providing the probability distributions of the EPBT and CO₂ emission factor, the uncertainty analysis provides valuable information reflecting environmental risks related to OPV projects for investors. Moreover, the sensitivity analysis indicates the influence of varying inputs on the outcomes, which suggests the direction for further investigation to control the uncertainties. By comparing the proposed OPV technology with four typical silicon-based and thin-film PVs in the aspects of EPBT and GHG emissions, we demonstrate the great potential of future OPVs in environmental sustainability.

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**Notes and references**

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