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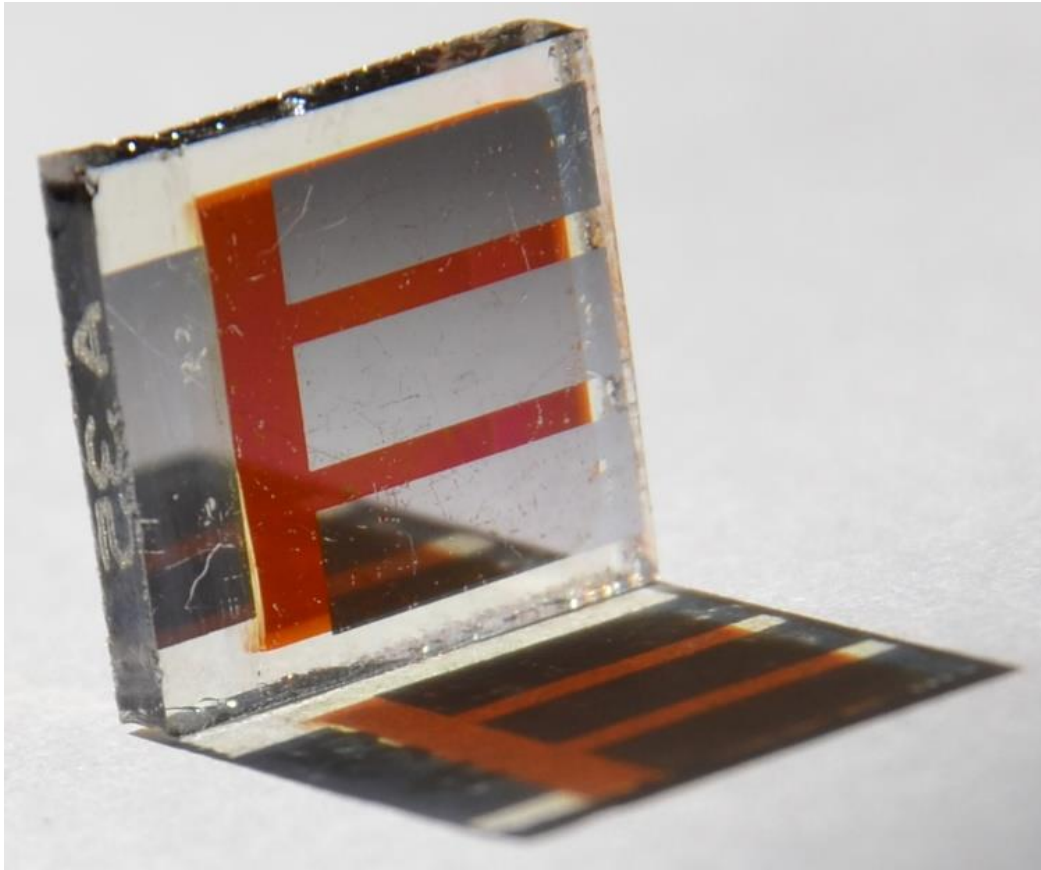

Life cycle assessment of perovskite solar cells and comparison to silicon solar cells

Master's Thesis within the Sustainable Energy Systems programme

JONAS STASIULIONIS

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Cover:
Sunlight shining through a solar cell incorporating a vapour-deposited perovskite absorbing layer. Picture credit: Phys.org

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ABSTRACT

The solar energy field has grown vastly in the past decades, and this trend seems to continue also in the future. But there is still a lot of work to be done in order to make solar energy competitive to other energy production systems. Because of this, there is constant research toward improving existing solar energy systems, and to find new materials to lower the initial cost and increase efficiency of energy producing units. Recently, a material called perovskite has received a lot of attention from the solar industry by potentially offering a cheap and efficient material for solar cell production. With efficiency increasing every year, this could potentially be the next dominant design for solar energy extraction. One of the main concerns brought up related to this new technology is the lead content of the perovskite solar cell. Because of the toxic nature of lead, and the potential of these cells to be produced in large quantities in the future, the possible impacts of lead to the environment have to be assessed.

This thesis consists of life cycle assessment of a perovskite solar cell and comparison to the currently most used common solar cell, which is the silicon solar cell. Several parameters were varied in the study in order to see which processes that have the largest influence to the environmental performance.

From the study, it was found that perovskite solar cells could be competitive with silicon solar cells from an environmental point of view if produced on a large scale. Management of lead use and emissions during the production process of perovskite cells had the largest impact on the results. If all of the lead used would be supplied from recycling, and emissions of lead from the cell itself during and after the use phase is completely prevented, perovskite cells show better environmental performance than silicon cells. Regarding manufacturing technology, the study showed that the blade coating technology is environmentally preferable over spin coating for large scale production of perovskite cells.

Key words: *Life cycle assessment (LCA), lead, toxicity, energy use, impact assessment*

Acknowledgments

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Jonas Stasiulionis

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Contents

Abbreviations

Ag-Silver

Al_2O_3-Aluminium oxide

Al-Aluminium

As-Arsenic

B-Boron

CaO-Calcium oxide

Cu-Copper

Fe_2O_3-Iron (III) oxide

Ga-Gallium

In-Indium

ITO-Indium tin oxide

K_2O-Potassium oxide

LCA-Life cycle assessment

MgO-Magnesium oxide

Mg-Magnesium

Na_2O-Sodium oxide

Ni-Nickel

P-Phosphorous

Pb-Lead

Pd-Paladium

SO_3-Sulfur trioxide

Sb-Antimony

SiO_2-Silicon dioxide

Si-Silicon

Sn-Tin

TiO_2-Titanium oxide

Ti-Titanium

1   Introduction

This chapter provides an overview of this study concerning its context, aim and main questions to be answered. The method that will be used in this study is also presented.

1.1   Background

The global energy demand is increasing and with the current goal set by the European Union (EU) to increase the share of the energy consumption from renewable energy sources to 20% by the year 2020, as pointed out by EU's Renewable energy directive (European Commission, 2015), the interest of utilizing solar power has been increasing (IPCC, 2007). Recently, a perovskite solar cell with lead-based absorber has received a lot of attention from solar cell producers since it offers the promise of relatively cheap and efficient solar cells (News Every day, 2015). In this study, the name *perovskite* refers to a material that has a same crystal structure as calcium titanium oxide ($CaTiO_3$), which is known as a *perovskite structure*. Some of these materials can be used to replace the current commercially used silicon in solar cells as an absorber of light, and as later noted, also as a conductor. Methylammonium lead tri-iodide ($CH_3NH_3PbI_3$) was the first absorber with the perovskite structure that was investigated for potential use in a solar cell (Peplow, 2014). Although relatively low efficiencies were achieved at the start, after a few years, efficiency values were achieved which could rival the commercially used silicon-based solar cells. The same production line as for silicon-based solar cells can also be used for production of perovskite solar cells. This means that some of the necessary manufacturing facilities are already in place, and thus brings promises that cheap production costs could be achieved relatively fast.

Although considered to be more efficient and cheap than the currently more common silicon-based solar cells in few years, the production of these cells could potentially be more environmentally damaging because of the lead content of the cell. Lead is toxic to humans and organisms in the environment, and its raw material acquisition has considerable environmental impacts (U.S. Environmental Protection Agency, 1994). Although the mass content of lead in a perovskite solar cell is not high compared to the mass of the whole cell, if implemented on a large scale, the demand for lead would grow and this could lead to high environmental impacts because of the high toxicity of lead and the polluting nature of its extraction process.

It should be noted that it is not always that a toxic heavy metal with high environmental impact in itself leads to similarly high life cycle impacts of products in which the metal is a constituent. One example is mercury in fluorescent light bulbs. According to Eckelman and colleges (2008), increased use of mercury-containing light bulbs does result in increased emissions of this heavy metal to the environment due to brakeage, incineration and subsequent evaporation. However, the use also leads to reduced electricity demand. If the avoided electricity is coal power, this reduced electricity demand results in avoided emissions from electricity production, where mercury is one of the emissions. As pointed out by Eckelman and colleges (2008), it is a complex task to assess and compare emissions of a particular substance from one application which is associated to energy systems, and the total energy production mix has to be taken into account. However, using energy-efficient light bulbs with mercury can lead to reduced net life cycle emissions of mercury.

Another example is cadmium in cadmium telluride solar cells. Emissions of heavy metals that occur throughout the life cycle of such solar cells have been shown to be small compared to emissions that are avoided from electricity production when these solar cell are integrated into the grid (Fthenakis et al., 2008). Whether the same environmentally beneficial situation is present for lead-containing perovskite solar cells has not been previously investigated.

1.2   Aim and research question

The aim of this study is to compare the environmental performance of perovskite solar cells to that of silicon-based solar cells. This is done in order to reveal which of the two solar cells that is more "environmentally friendly", that is, has lower environmental impacts. The comparison is made with the respect to the functional unit of the study which is 1 kWh of produced electricity. The research question can be stated as: Which of the two solar cells has lower environmental impact throughout its life cycle (cradle-to-grave)?

1.3   LCA method

The life cycle assessment (LCA) method is used in this study to compare two different solar cell technologies. This method is used to quantitatively assess the environmental impacts of a product or service on the environment. It takes into account all the material and energy flows throughout the lifecycle of a product (cradle-to-grave). The emissions and resource use of all processes, from raw material acquisition to final disposal, are included and then quantified in terms of a functional unit. Usually, LCA includes the goal and scope definition, inventory analysis, impact assessment and interpretation phases (Baumann and Tillman, 2004). There are several international standards for LCA, and one of them, ISO 14040 (2006), defines LCA as a technique for assessing the environmental aspects and potential impacts of a product by collecting data of all inputs and outputs of the system, associating environmental impacts to those inputs and outputs, and summarizing these impacts in accordance with the goal and scope of the study (Baumann and Tillman, 2004). This method provides valuable information on possible process modifications that can be made in order to make the product more "environmentally friendly". LCA is often used to compare two or more products, or several options on how to produce or dispose of a product, in order to identify most preferred option from an environmental point of view. LCA was also the method used in the previously mentioned studies of the mercury-containing light bulb and the cadmium-containing solar cell (Eckelman et al. 2008, Fthenakis et al. 2008).

2 Technical description

This chapter provides the background for the use of solar energy, covers the working principle of solar cells and describes two different solar cells – silicon and perovskite solar cells. It also describes environmental and health aspects of lead.

2.1 Solar energy

The amount of energy that reaches the Earth in a form of light would be more than enough to supply all the electricity demand globally (IPCC, 2007). One way to utilize this incoming energy is to use photovoltaic technology (PV) that converts light into electric energy. The application of this technology is in the form of solar cells, where different kinds of semi-conductive materials are used for the production of electric power. This technology has a lot of applications, from small scale electric appliances, watches, and laptops, to larger scale electricity production in solar photovoltaic plants. However, the efficiencies of solar cells typically only reach 15-20%. Solar cells with higher efficiency can be reached but they are currently only on laboratory scale and not feasible for large scale production (NREL, 2015). To use it for large scale electricity production, one has to take into account the possible environmental impacts that would come from mass production of solar panels.

Because of the potential of being a relatively clean energy source, there is a constant search for new ways to increase efficiency and production rates of solar photovoltaics. In order to help this technology to develop further, governments are also involved, by subsidizing solar photovoltaics to support the use of such non-fossil energy sources (Hjalmarsson, 2014). This cooperation of researchers and governments can lead to an increase use of photovoltaic technology, and help in meeting the constant rising energy demands.

2.2 Efficiency of a solar cell

Not all light that reaches a solar cell can be used for electricity generation. The ability to induce electric current in a solar cell depends on the wavelength of the sunlight and the band-gap of the semiconductor material. The term *band-gap* here refers to the amount of energy required to increase the energy of the electron and free it from its valance position in the atom shell (Four Peaks Technologies, 2011). Photons with lower energy than the band-gap will go through the cell without exciting any electrons. Photons with higher energy levels than the band-gap will free an electron, but because of the excess energy, the rest of the energy will be lost as a heat (Four Peaks Technologies, 2011). The ratio of the light energy which is able to induce electric current in the cell, with the total light energy that reaches the cell, is referred to as the efficiency of a cell.

The first efficiency limit for the single junction silicon solar cell was calculated by William Shockley and Hans Queisser in 1961 under so-called standard test conditions (Four Peaks Technologies, 2011). It was called the Shockley-Queisser limit and had an original value of 30%. Standard test conditions are the test conditions used to test and compare different types of solar cells. These conditions are (Florida Solar Energy Center, 2010):

- Solar irradiation of the surface: 1000 W/m^2

- Temperature of the solar cell (not of the surrounding environment): $25 \pm 2°C$

- Air mass ratio: 1.5. The air mass ratio stands for the ratio of the actual distance of the solar radiation to the surface, to the vertical distance that the radiation travel to the sea level.

The current Shockley-Queisser limit for any type of single junction solar cell is 33.7 % (Four Peaks Technologies, 2011). Four main assumptions were made to apply this Shockley-Queisser limit to all types of solar cells (Florida Solar Energy Center, 2010):

- Only one semiconductor material in a solar cell

- Only one p-n junction

- The irradiance of the sun is dispersed unequally over the solar cell surface

- Photons that have a higher value than the semiconductors band-gap are converted into heat.

There are few strategies suggested by Four Peaks Technologies (2011) to potentially exceed the Shockley-Queisser limit:

- The use of several semiconductors in the cell

- Implementing more than one p-n junction

- To concentrate light to the solar cell

- Implementing combined electricity and heat generation.

2.3   Silicon-based solar cells

There are several types of solar cells, but the majority currently used are wafer based crystalline silicon PV (Chu, 2011). This includes both single-crystalline and multi-crystalline silicon cells. As reported by Chu (2011), other commonly used PV panels are thin film panels, which include cadmium telluride (CdTe) and copper-indium-gallium-diselenide (CIGS) panels. Since the silicon-based solar cells are the most common type of cells being used today, this type of cell was chosen for comparison to the perovskite solar cells in this study.

Figure 1 shows a categorization of solar cells based on the main active material. Currently, the crystalline silicon material is dominating the market, with the largest share coming from polycrystalline silicon (Dobrzanski et al., 2012). The solar cells containing perovskites, which are studied in this thesis, are part of the organic structure group of solar cells, which currently only holds a minor share of the market.

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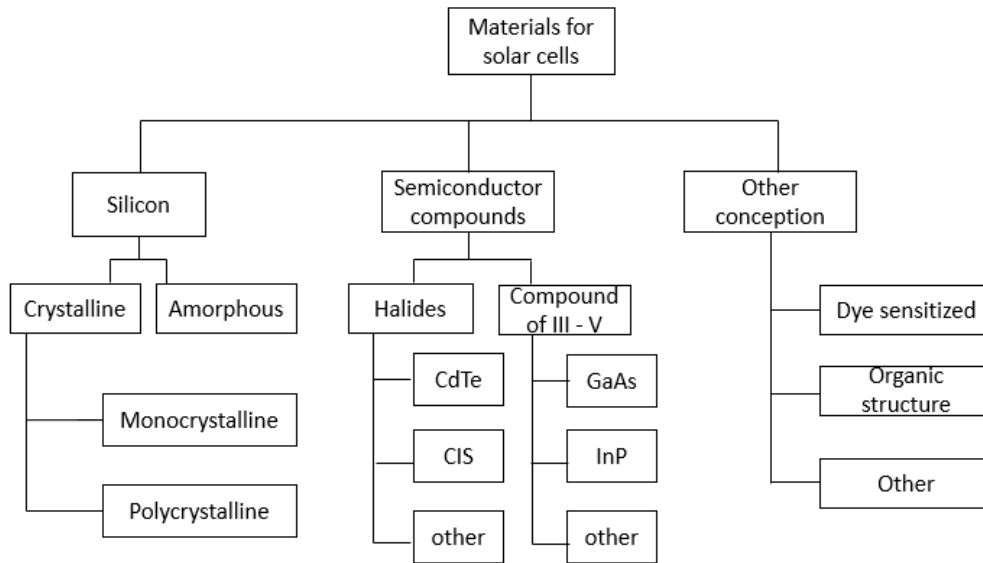
Figure 1.   Categorization of solar cell materials. Modified from Dobrzanski et al. (2012).

2.3.1   Working principle

As mentioned previously, the polycrystalline silicon-based solar cell is the dominant design on the market today. For this reason, the working principle of this cell will be presented in this section.

Solar cells use the photovoltaic effect to convert the energy of light (photons) into electric energy. This is achieved when a photon causes the release of an electron from a semi-conductive material. For the polycrystalline silicon cells, silicon is used as a semi-conductive material.

A silicon atom has four valance electrons, which bind to atoms next to it. These four electrons are the only ones that can interact with the neighbouring atoms. Pure silicon, found in nature in the form of silicon dioxide (quartz), has a low value of electric conductivity. To increase its conductivity, silicon is doped with other materials. The term doped means that a material is intentionally contaminated by another material. In this case, phosphorous and boron are added to the silicon crystal structure to make it a p-type or an n-type semi-conductor (Four Peaks Technologies, 2011). Silicon infused with phosphorous is called n-type (n stands for negative) because of the excess of electrons (Aldous et al., 2007). The excess of electrons results from the different number of electrons in the outer shell of silicon and phosphorous atoms. Phosphorous has five electrons in its outer shell, which compared to four electrons of silicon, leaves one extra electron, which requires less energy to be set free. Silicon infused with boron is called p-type (p stands for positive) because of the excess of "electron holes" (Aldous et al., 2007). There are three electrons in the outer shell of the boron atom, which in combination with silicon atom leaves a "hole" in the form of an absent electron.

In the solar cell, these two silicon types are put next to each other. Free electrons and holes mixes together to form a p-n junction – a one-way barrier for the free electrons. This barrier allows movement of electrons only from the p-layer to the n-layer, a one-way movement of electrons – electric current (Aldous et al., 2007).
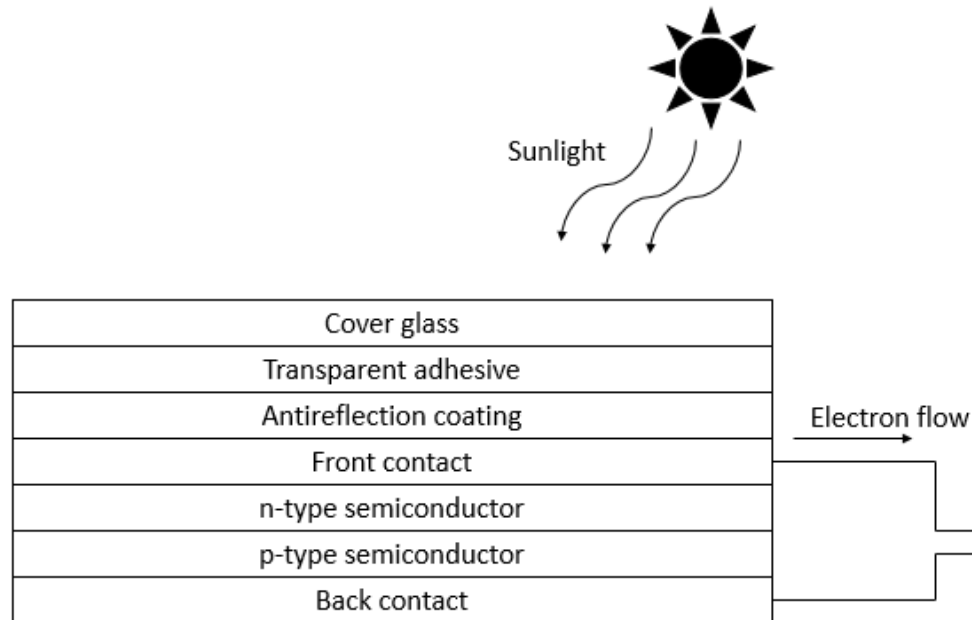
Figure 2.   Crystalline silicon cell structure. The size of the components in the figure do not represent their actual size in a real cell. Modified from Four Peaks Technologies (2011).

Figure 2 shows a typical structure of a crystalline silicon cell. It can be separated into seven main layers:

1. Cover glass. Functions as a protective layer for the other parts of the solar cell. The glass is usually chosen to have a high solar energy transmittance, to allow a maximum absorption of a solar energy in the underlying layers. For the crystalline solar cells, the cover glass is often already combined with an antireflection coating layer (Pilkington, 2014).

2. Transparent adhesive. This layer functions as an additional protective layer and as a bonding material between the solar cell and cover glass. Silicon-based rubber materials are usually used (Yuan, 1982).

3. Antireflection coating. Bare silicon has a reflection index of over 30% (Tobias, 2005). This means that a special coating material over the semi-conductive layer is required in order to increase the efficiency by reducing the amount of sunlight reflected away from the solar cell surface. The antireflection coating is a non-absorbing, conductive material used to reduce the reflection of the solar cell. The thickness of this layer is specifically designed to exploit interference effects of waves reflected from different layers of the cell, which could otherwise interact in a destructive manner, resulting in lower efficiency (Tobias, 2005).

10

4. Front contact. Contacts are made of conductive and transparent materials, and serve as connection materials between the solar cell and the external circuit. For silicon cells, indium tin oxide (ITO) is usually used as front contact material (Tobias, 2005).

5. N-type semiconductor. Silicon doped with phosphorous. This layer has an excess of free electrons, because of a higher number of electrons in the outer shell of phosphorous relative to silicon.

6. P-type semiconductor. Silicon doped with boron. This layer of the solar cell has an excess of electron holes, because of a higher number of electrons in outer shell of boron relative to silicon.

7. Back contact. Same as the front contact, the back contact functions as a conductor of electric current and provides support for the structure of the solar cell. Silver or gold can be used as the materials for the back contact.

A solar PV cell is the smallest device that converts sunlight into electricity (Figure 3). These cells are structured into modules in a formation that depends on which characteristic is required to improve (current or voltage). A solar panel is a collection of solar modules on a structure. Arrays are usually used in solar PV plants for large scale electricity production and consist of compilations of solar panels (Sidhu and Carlson, 2010).
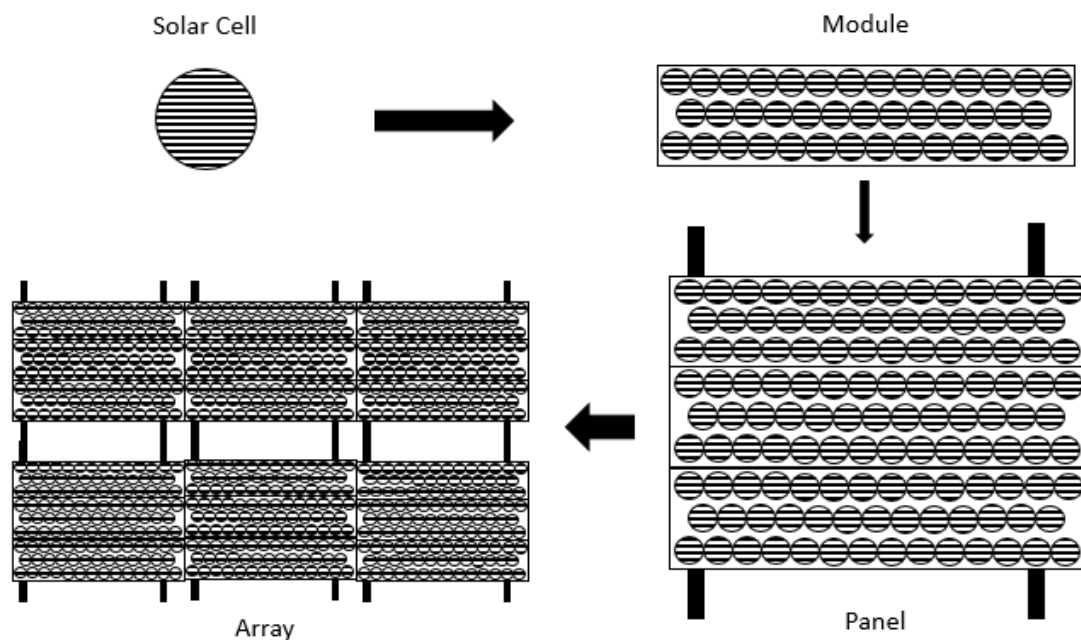
Figure 3.   Composition of solar technology from cell to array. Modified from Solar Direct (2014).

The materials used and their approximate mass percentage in a solar module are presented in Table 1, as reported by Goetzberger (2005). As can be seen from Table 1, glass is the part that contributes the most in terms of mass. It can also be noted in Table 1 that a very low mass of materials for doping are required.

Table 1.   Materials contained in solar module. Possible material alternatives are presented in brackets. Modified from Goetzberger et al. (2005).

Components	Materials used	Approximate mass percentage without frames (%)
Glass (2-10 mm)	SiO_2, Al_2O_3, Fe_2O_3, CaO, MgO, Na_2O, K_2O, SO_3	30-65
Transparent adhesive (1-2 mm)	Ethylene vinyl acetate , acrylate	5-10
Semiconductor (200-400 µm)	Silicon	5-10
Connection material (0.04×2-0.2×5)	Cu [Sn, Pb, Ag], Al [Mg, Si]	1
Metallization	Ag, SiO_2, Cu, Ni, Al, Ti, Pd, Sn	< 0.1
Antireflection layer	TiO_2	> 0.1
Doping	B, P [Al, Ga, In, As, Sb]	<< 0.1
Cable 1.5-2.5 mm^2	Cu, polyvinyl chloride, rubber, silicon, polytetrafluoroethylene	1
Connection box	Acrylonitrile butadiene styrene , polycarbonate , polyvinyl chloride (, Cu, brass, steel, rubber	0-5
Sealing, gum	Silicone, polysulfide, cyanacrylate	0-10
Back side material	Chlorofluorcarbon, polyster	0-10

2.4   Perovskite solar cells

In recent years, a new material for photovoltaic technology has received increasing attention from researchers and solar cell producers (Loi et al., 2011). Materials called perovskites have begun to be used as absorbents of light, and even as charger carriers. The name perovskites refers to a group of materials that share the same crystal structure as calcium titanium oxide (Science Daily, 2014). These types of solar cells offer relatively high efficiencies that have been increasing dramatically in a few years. With an increase in efficiency from 3.8% to nearly 20% from year 2009 to 2014, this is the

fastest growing solar cell technology today (NREL, 2014). The most notable drawbacks of this technology is the lead content of the cell, and solar cell durability, which is currently too short for large scale implementation.

2.4.1 Working principle

Most efficient perovskite solar cells today have a similar working principle as the thin film solar cells. Currently, the most commonly used absorber in perovskite solar cells is methylammonium lead trihalide (Peplow, 2014). For this reason, this study will focus on this perovskite material.

The first models of perovskite solar cells were based on the structure of dye-sensitized solar cells, where organic materials were deposited over a porous TiO_2 layer (Loi et al., 2013). Later studies showed that perovskite layers can also transport electrons and more simple designs, based on the thin film solar cell structure, were developed (Loi et al., 2013). Several studies trying to achieve higher efficiencies for both designs have been, and are still being, conducted. Figure 4 shows two types of perovskite solar cell designs. A dominant design with highest efficiency and best performance has not been established yet (Jiandong et al, 2014).

The main difference between these two designs is how the perovskite layer is used. In a hybrid sensitized solar cell, the perovskite acts only as a light absorbent, and other materials are accountable for the charge carrier function (Loi et al., 2013, Figure 4a). An alternative structure, similar to the thin film architecture, was proposed when it was found that perovskites can act not only as absorbents of light, but also as charger carriers (Figure 4b).
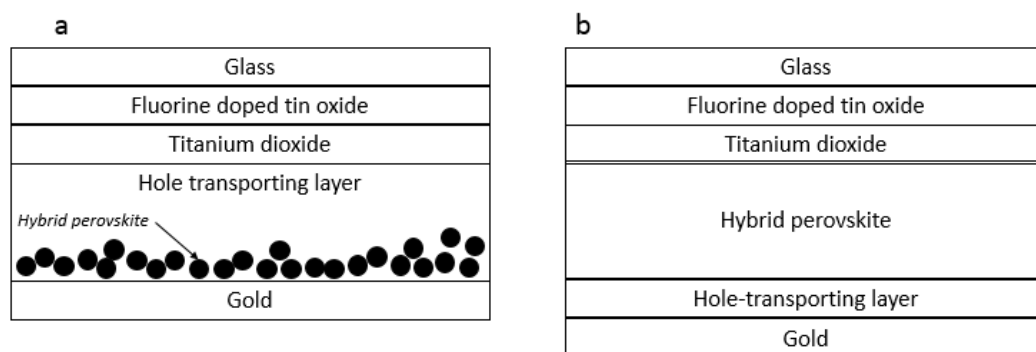
Figure 4   Architectures of perovskite solar cells. a: Hybrid sensitized solar cell. b: Planar hybrid thin film solar cell. Modified from Hummeln et al. (2013).

For the purpose of this study, planar hybrid thin film perovskite solar cell (as in Figure 4b) with Spiro-OMeTAD hole transmitting layer will be investigated due to its relatively simple design and more accessible data for the study. The manufacturing process for this type of solar cell is a solution-based, vapour-assisted process (Jiandong et al., 2014), which will be discussed in later sections. The basic structure of a planar thin film perovskite solar cell is presented in Figure 5, with basic functions of each layer shown:
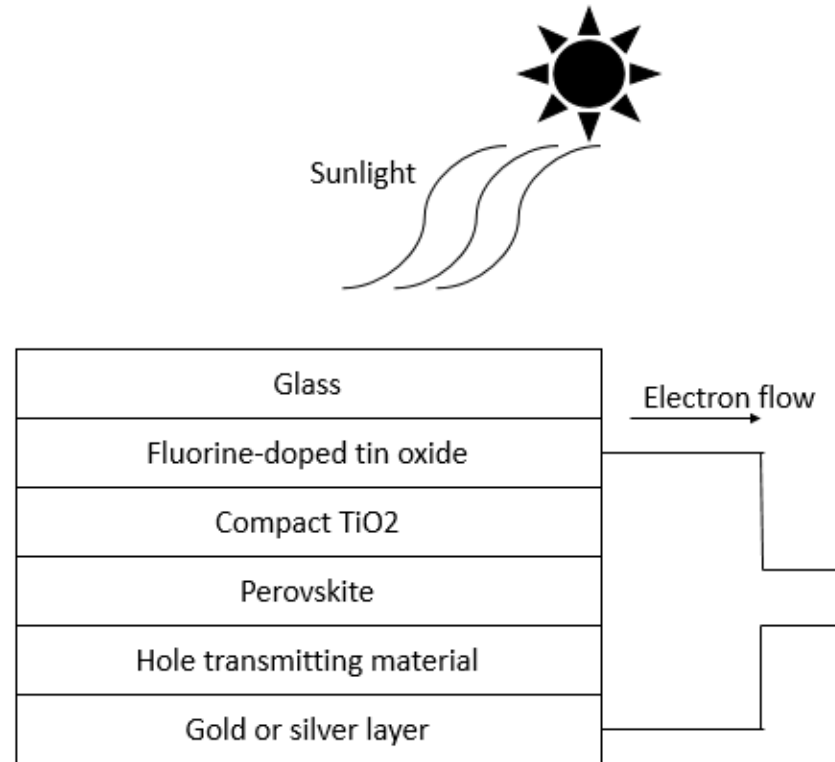
Figure 5   Structure of a perovskite solar cell. The sizes of cell components in the figure do not represent actual component sizes. Image modified from: Green et al., 2013.

1. Glass layer. As for the most of the solar cells, the top glass layer functions as protection for other parts of the solar cell.

2. Fluorine-doped tin oxide (FTO). Electrically conductive and transparent coating layer on top of the glass layer. Used in a wide range of applications, fluorine-doped tin oxide performs well in solar cells because it is stable under atmospheric conditions, resistance to high temperatures, and cheaper than indium tin oxide, which is another material that can be used for the same function (Sigma-Aldrich, 2015).

3. Compact TiO_2. This semiconducting layer functions as an electron charge absorber and charge carrier.

4. Perskovite. The main layer for light absorbtion, and in some designs it functions also as a charge carrier.

5. Hole transmitting material. For this study, the material used is Spiro-OMeTAD. It is an organic hole carrier material, in which the electric conductivity depends on uncontrolled oxidative process (Nguyen et al., 2015).

6. Gold or silver layer. Highly conductive layer of gold or silver for the extraction and transportation of electrons.

14

2.5   Tandem silicon-perovskite solar cells

As mentioned above, crystalline silicon solar cells are currently dominating the solar cell market. While the production costs for these cells have been gradually decreasing, the efficiency of these cells has remained constant at around 24% for more than ten years (NREL, 2015). Because of already existing factories, relations between manufacturers, implemented policies, and low production costs, it is hard for new technologies to enter the market (Dobrzanski et al., 2012). For this reason, the enhancement of the efficiency of the currently dominating silicon solar cell is of a great interest.

One way to achieve this is the combination of two solar cells with different properties in order to reach higher total efficiency of the whole solar cell. The main task to consider when combining two solar cells is to choose materials with specific levels of band-gaps. The target is to have a solar cell with a higher band-gap on the top in order to maximize the light absorption (Bailie, 2014). A main barrier here is the lack of available materials for the top part of the solar cell, which should have a high band-gap. However, with the introduction of perovskite materials as photovoltaic technology, this has opened new possibilities in the tandem solar cell field.

The increased efficiency of tandem solar cells compared to solar cells with only one light-absorbing material can be explained by Figure 6. In a silicon solar cell, which has a band-gap of approximately 1.4 eV, photons with equal and lower energy are absorbed and converted into electricity. Photons with higher energy are also absorbed, but due to their high energy, they are dispersed as heat in a cell. In a tandem solar cell, photons with energy higher than 1.4 eV are absorbed and converted into electricity by the top cell, which has a higher band-gap than the silicon one (around 1.6 eV). The photons with equal or lower energy than 1.4 eV are absorbed and converted into electricity in the bottom cell in the same way as for a silicon-only solar cell.

A combination of a silicon cell or a copper indium gallium diselenide cell with a hybrid perovskite solar cell was proposed by Bailie et al (2014). According to them, the band-gap of a top cell should preferably be 1.7-1.8 eV, which makes perovskite cell a good candidate for the top cell, having a band-gap around 1.6 eV.
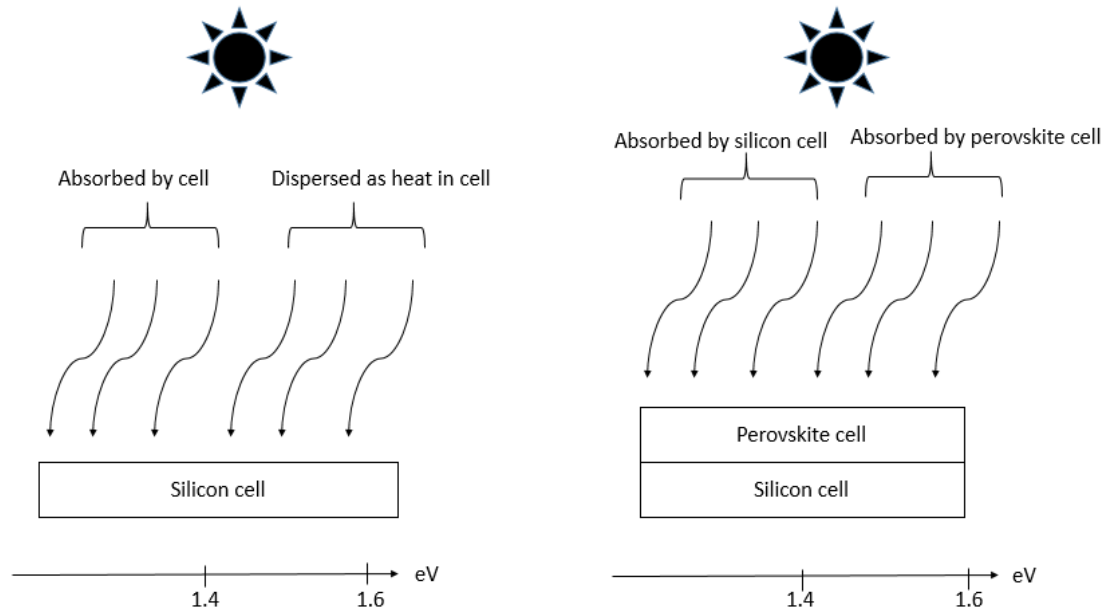
Figure 6   Photon absorption principle for single silicon solar cell (left) and for tandem solar cell (right).

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2.6   Lead toxicity

Since one of the main barriers for implementing perovskite solar cells on a large scale is uncertainty about environmental effects from the production, especially related to the lead content, it is important to know and understand the consequences that high exposure of lead can have for human health and the environment.

Although lead is a naturally occurring metal, most of the lead concentrated in the environment comes from human activities (USDHHS, 2007). Such activities include mining, burning of fossil fuels or municipal waste, combustion of fuel in vehicles and disposal of car batteries without recycling. Once released into the environment, lead cannot be degraded by natural means, only changed into other forms of lead (US DHHS, 2007).

According to the World Health Organization (WHO), there are several ways for humans to be exposed to lead: breathing air containing lead particulates, drinking water and eating food or accidentally swallowing dust with lead content. There is particularly high risk for people living close to mining industries or high-intensity highways.

Children and pregnant women are the group with highest risk of effects from exposure to lead, since the body of the child or infant is still forming and growing. The WHO has set tolerable lead intake levels based on a scientific review conducted in 2010: 1 µg/dL of lead in drinking water, and 0.5 µg/m^3 lead in air (WHO, 2010). The US Environmental Protection Agency has set up guideline values for lead exposure according to Table 2.

Table 2.   Hazardous exposure doses of lead for different social groups (numbers presented in micrograms per decilitre in blood). Table developed from the US Environmental Protection Agency (2012).

Lead exposure dose	Consequences for different social groups
100-150 µg/dL for less than 14 days	Children: death Adults: brain and kidney damage
15-30 µg/dL for less than 14 days	Increases blood pressure in middle aged men
10-15 µg/dL for less than 14 days	Pregnant woman: reduces birth weight and mental ability of infants
15-20 µg/dL for more than 14 days	Children: reduces growth rate
10-15 µg/dL for more than 14 days	Pregnant woman: greatly reduces birth weight and mental ability of infants

An excessive amount of lead in air or soil can be dangerous not only to humans, but also to animals and local ecosystems. Lead pollution can cover the surface of plants and prevent them from absorbing light or reducing the rate of photosynthesis required for plant to function, thus leading to reduced growth rate or killing the plant (Greene, 1993). Some of the plants are more resistant to lead exposure which could result in a complete change of local ecosystem, with an extinction of less resistant plants and microorganisms. According to the US Environmental Protection Agency, a regular intake of 2-8 mg of lead per kilogram of total body mass over an extended period of time will result in death for most animals (Greene, 1993).

3 Goal and scope

This chapter describes goal and scope definition, including definition of system boundaries.

The goal of this study is to compare two types of photovoltaic solar cells – silicon-based solar cells and perovskite solar cells, and to investigate which of the two that has the lower impact to the environment throughout its life cycle. Since perovskite solar cells is a new technology, which is not available on the market yet, this study is a prospective LCA (Sandén and Karlström 2007). In that sense, it is similar in scope to other conducted prospective LCA studies, for example Arvidsson et al. (2015).

3.1 Functional unit

The functional unit of this study is 1 kWh of produced electricity from the solar cells, since the purpose of solar cells is to produce electricity. This functional unit has also been used in previous LCA studies of solar cells (Jungbluth, 2005, Alvebratt and Blidmark, 2014). Ideal condition for solar power production, which is 1000 W/m^2 of surface solar irradiation, is assumed in this study, which means that the solar cells produce at maximum of its capacity.

3.2 System boundaries

A cradle-to-grave perspective is applied in this study. It includes all processes from raw material acquisition to the final disposal. Comparative, attributional LCA is used in order to determine and compare the energy use and emissions from the two solar cells. The cradle-to-grave approach in LCA studies is presented in Figure 7.
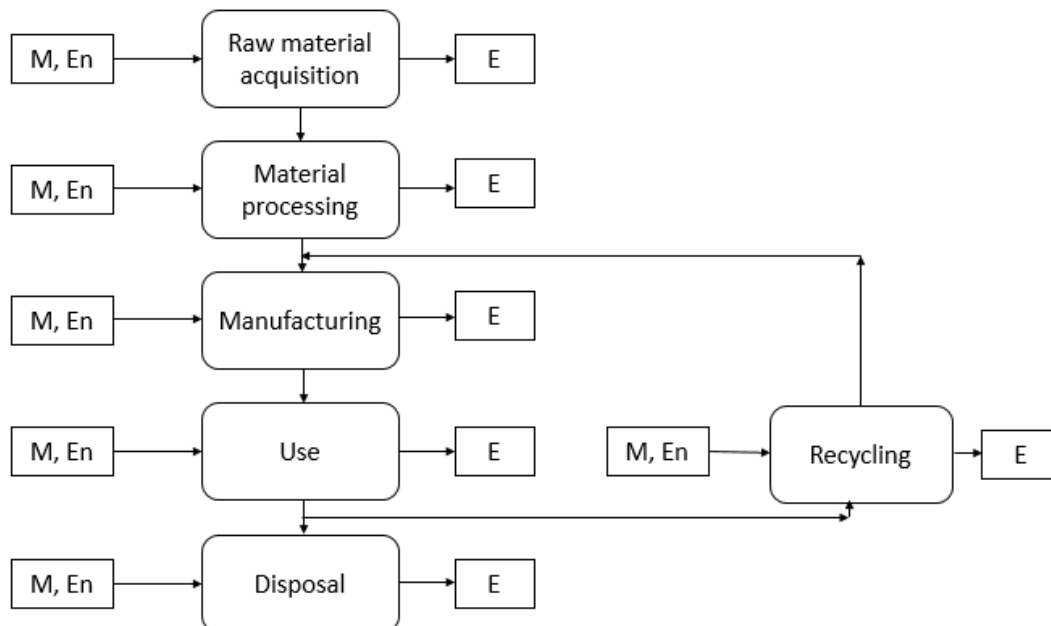
Figure 7   Cradle-to-grave approach of product LCA. M: Material input, En: Energy input, E: Emissions from the process.

A product system can be divided into foreground and background systems (Baumann and Tillman, 2004). Such a division is done in the study. In the foreground system, all the processes for the production of main components of the solar cell are included. In the background system, production of electricity and heat are included. The division into foreground and background systems for the production of the solar cells is shown in Figure 8.
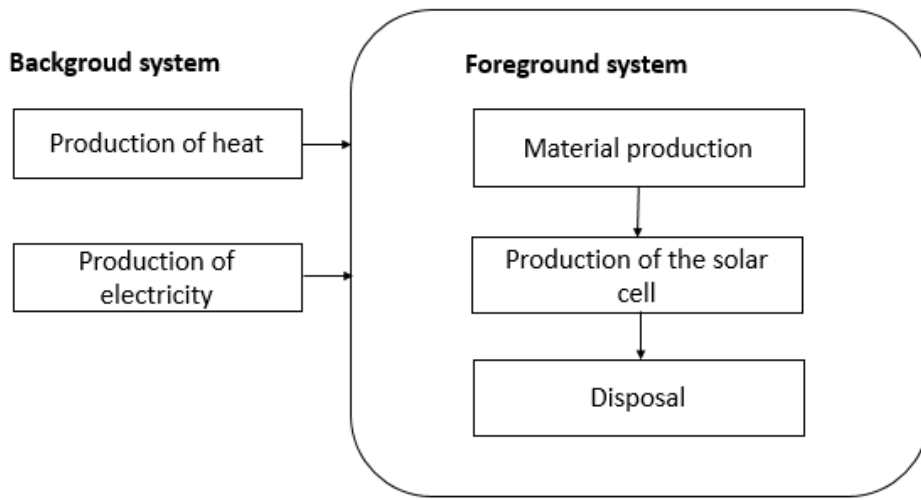

Figure 8.   Division into foreground and background systems in the production of solar cell, as conducted in this study.

3.3   Impact categories and impact assessment methods

For this study, impact categories that lead contributes to, such as human toxicity and ecotoxicity, are included. The reason for this is that lead is a crucial constituent for one of the solar cells, and that lead has high environmental and human health impacts (see section 2.6). Energy use is also investigated in the study, since the purpose of a solar cell is to produce energy, and high energy demand during the production of a cell would be problematic. Toxicity from the production of energy (i.e. the background system, see Figure 8) is also included in the calculations, and results are presented as total toxicity for both solar cells. Impact categories that are used in the study are listed and described in more detail below:

- Human toxicity potential. This impact category includes emissions of substances that are hazardous to human health. Heavy metal emissions contribute largely to this impact category. In this study, two different toxicity assessment methods are used considering the challenges of assessing toxicity in LCA (Finnveden et al., 2009). These are the USES-LCA method and the USEtox method. In USES-LCA, human toxicity potential is expressed using a reference substance, 1 kg of 1,4-dichlorobenzene (Huijbregts et al., 2000). The

USES-LCA impact assessment method is used here because it is an established method as a part of the ReCiPe impact assessment method (Goedkoop et al., 2008). USEtox is chosen because it is the most recently developed consensus model for toxicity assessment in LCA. The unit of measurement in USEtox is comparative toxic units (CTU_h), which describes the increased morbidity for the human population per kg of chemical emitted (Hauschild et al, 2008). Two impact assessment methods are chosen to compare and check the robustness of results.

- Ecotoxicity. This impact category characterizes all emissions to air and water that are hazardous to organisms in the environment. It includes emissions that are associated with decreasing local biodiversity and wildlife. Again, two different toxicity assessment methods are used: USE-LCA and USEtox. The results from USES-LCA are expressed relative to 1 kg of 1,4-dichlorobenzene (Huijbregts et al, 2000). In USEtox, results are expressed as cumulative toxic units for the environment (CTU_e), which translates to the change in potentially affected fraction (PAF) of species for the change in chemical concentration occurring due to the emission.

- Energy use. This impact category accounts for the use of energy. The unit of kWh is chosen to match the functional unit, which is also expressed in kWh. The total energy is divided into thermal energy (kWh_{th}) and electrical energy (kWh_{el}). Such a separation of energy between heat and electricity was also conducted by Kushnir and Sandén (2008) in order not to aggregate these two entropically different types of energy.

3.4   Sources and software

Information about the production of silicon cells is obtained from two different LCA studies – one by the International Energy Agency (Fthenakis et al., 2011) and one by the Swiss Ecoinvent database (Jungbluth, 2004). Available process data for the production of perovskite solar cells were collected from an article in the journal Nanoscale Research Letters (Chen, 2013). Data for the processes is gathered from the online Unit Process Data (UPD) database Ecoinvent version 2.2 (2010). For the toxicity impact assessment, two sources describing the applied methods were used: Huijbregts et al., 2000 for USES-LCA and Hauschild et al (2008) for USEtox.

4   Life cycle inventory for silicon cells

In this chapter, the inventory modelling and data collection for the silicon cell is described. This data is subsequently used for impact assessment.

4.1   Initial flowchart of the process

Figure 9 shows the process flow chart for the production of silicon solar cells. The production processes are described in more detail in subsequent sections.
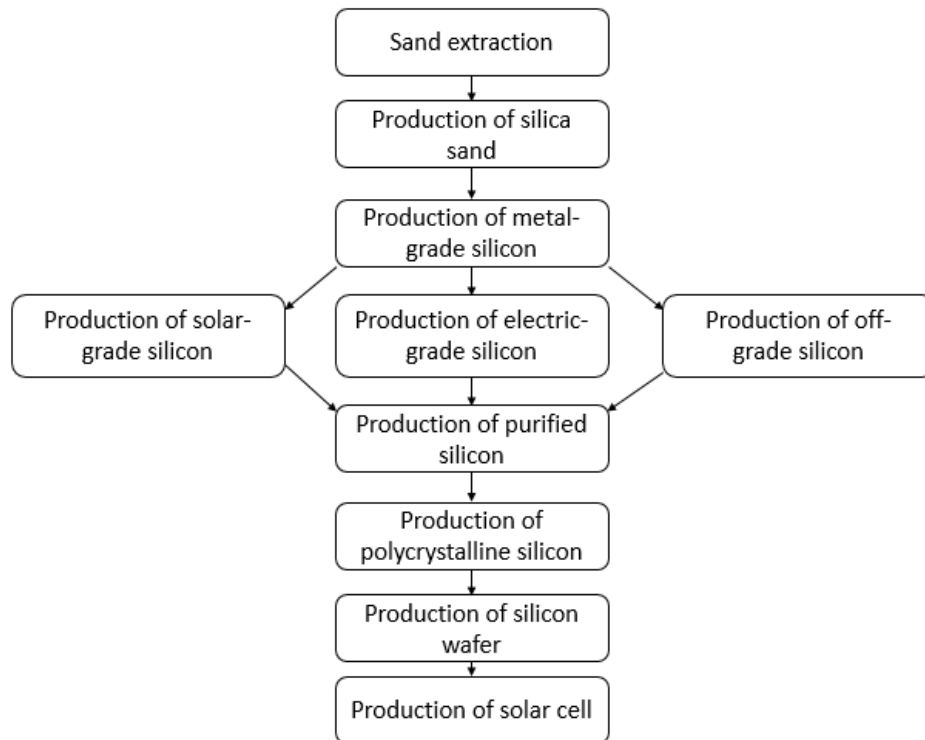
Figure 9   Flowchart for production of silicon photovoltaic solar cell.

4.2   Sand extraction

Unit Process Raw data is obtained from the Ecoinvent database–"sand, at mine" (#478). The process represents production in China and inputs to the process are electricity and burning of the light fuel oil in industrial boiler. The land use for the mine and the manufacturing of the operation machinery are excluded from the study.

4.3   Production of silica sand

Production of silica sand includes drying of the sand and removing impurities and other materials to achieve high purity silica sand. The main energy input into process is heat for the drying of the sand, produced by burning light fuel oil at industrial furnace. This process is described in the Ecoinvent database "silica sand, at plant" (#479), and relevant inventory data is available. The data represent production in China.

4.4 Production of metallurgical-grade silicon

The so-called carbothermal reduction process is used for the production of metallurgical-grade silicon (MG silicon) from the silica sand (Jungbluth, 2005). The process inputs consist of electricity input from the local grid, use of reducing agents such as charcoal, petroleum coke, and hard coal, and some minor inputs of chemicals such as liquefied oxygen and graphite. The production of reducing agents and chemicals, which are used in the process, and the energy use for these processes, have been taken into account. For the production of these products, electricity is the major energy input, as specified by the Ecoinvent data set "MG-silicon, at plant" (#1112).

4.5 Solar-grade, electric-grade, and off-grade silicon production

To be able to use silicon in photovoltaic technology, it has to be purified to a higher level of purity than MG silicon. Three processes from the Ecoinvent database describe this: "Silicon, solar grade, modified Siemens process, at plant" (#1194), "silicon, electronic grade, at plant" (#1190), "silicon, electronic grade, off-grade, at plant" (#1191).

The solar-grade silicon is produced using the so-called modified Siemens process, which uses less electricity compared to usual Siemens process. In the Siemens process, high-purity silicon is produced in a vacuum chamber using high temperature as the nucleation state for silicon deposition (Aldous, 2007). This high-purity silicon is deposited on thin polysilicon rods via vapour deposition process. The demand for process electricity and heat is covered by natural gas-fired cogeneration plant.

Production of electric-grade and off-grade silicon share the same process input and outputs as the solar-grade silicon. A silicon production mix consisting of all these three products is used in the further production chain. For the production of 1 kg of silicon to be used in solar cell production, 0.80 kg is of solar-grade silicon, 0.15 kg is electronic-grade silicon, and 0.05 kg off-grade silicon, as stated in the Ecoinvent data set "Silicon, production mix, photovoltaics, at plant" (#6874). The difference for these three products is the purity of silicon, where electric-grade silicon has the highest purity.

4.6 Production of polycrystalline silicon block

At this point, the purity of the silicon is high enough for solar cell production. The next step is the melting of the purified silicon and casting it into forming boxes. After the right form is obtained, the edges of the silicon blocks are cut off and blocks are formed. For this process, the only energy input is electricity. Other inputs consist of some chemicals and ceramic tiles. The ceramic tiles are used to store and form the melted silicon into block formation. Chemicals used in the process include liquid nitrogen and argon. Emissions and energy use for production of these tiles are included in the process "production of polycrystalline silicon block" (#1192) described in the Ecoinvent database.

4.7   Production of silicon wafers

The silicon block is sawn into 240 µm thick and 156×156 mm^2 size wafers. In the data set from Ecoinvent, "multi-Si wafer, at plant" (#6826), the reference flow is 1 m^2 of wafer surface. Inputs to the process include electricity, water use and consumption of some materials, which include some chemicals for cleaning and etching the wafers, as well as wire drawing and steel for cutting the wafers.

4.8   Production of solar cell

Parameters for the produced solar cell are as follow: 156×156 mm^2 size, 270-300 µm thick solar cell, with an efficiency of 13.5% and 1.3 W power capacity. In the Ecoinvent data set, "photovoltaic cell, multi-Si, at plant" (#6828), the reference flow is production of 1 m^2 solar cell. After purification and etching of the wafers, they are doped with n-type and p-type materials. Thin layers of antireflection coating and transparent adhesive are added in this process section. Due to their low contribution to the total mass of the cell, and to the total emissions, these components are not represented separately in the flow chart, but are included in process production of solar cell. Finally, the front and back contacts are added to the cell. Production of the front and back contact paste have electricity and heating from natural gas as a main inputs to the process. Inputs to the process include electricity, chemicals and some additional components like metallization paste for front and back contacts.

4.9   Transportation

Considering the prospective nature of this study, future production locations and transportation distances cannot be known with certainty. In order to still investigate the potential contribution to toxicity and energy use from transportation, a hypothetical transport scenario was derived based on the Ecoinvent data and is presented in Table 3. Transport distances by sea and road are calculated using SeaRates calculator (www.SeaRates.com). In this source, the speed of ships from China to Europe is reported to be approximately 14 knots, which is similar to the speed of large ship according to the classification by Baumann and Tillman (2004).

For the land transportation, Euro 5 class medium sized distribution trucks are assumed. Euro 5 class trucks are chosen because of the emission regulations that apply to transportation, and Euro 5 class trucks are the most recent ones to satisfy these regulations according to emission standards by European Union (TransportPolicy, 2014). The Euro 6 class is already existing, but implemented only recently.

Table 3.   Hypothetical locations of production processes of silicon photovoltaic cell.

Process	Hypothetical locations
Sand extraction	China
Silica sand production	China
Metal-grade silicon production	Europe
Solar-grade, electric-grade, and off-grade silicon production	Europe
Multi casted silicon production	China
Silicon wafer production	China
Photovoltaic cell production	China

The data for emissions for truck transportation include fuel consumption, emissions and energy requirements for the production of fuel (Baumann and Tillman, 2004). Emissions of large ship and truck transportation are calculated based on the data in Table 4. The environmental impacts of construction of vehicles, roads and other infrastructure are not included.

Table 4.   Emissions from large ship transportation and medium sized class distribution truck transportation (Baumann and Tillman, 2004).

Energy requirement and emissions [MJ/t km or g/t km]	Large ship	Medium sized distribution truck, Euro 5 class
Energy	0.22	1.9
CO_2	15	2.3
NO_x	0.43	0.082
HC	0.020	0.11
Particulate matter, PM	0.020	0.005
CO	0.0087	0.12
SO_2	0.26	0.034

4.10   Electricity production

Since the object of this study is to compare two products, where one is not implemented on the market yet, a general approach to electricity production was implemented in order to account for future changes in electricity production and different potential geographical locations. Electricity production was based not on the specific mixes reported in the Ecoinvent database, but instead varied in the sensitivity analysis. For the baseline scenario, the Swedish electricity mix was chosen, where approximately half of the electricity is produced from nuclear power and the other half from hydro power. This electricity mix represents one with low toxic emissions. One scenario with only coal power, and one with half coal and half natural gas, were also assessed.

5 Life cycle inventory for perovskite solar cell

In this chapter, the inventory modelling and data collection for the perovskite cell is described. This data is subsequently used for impact assessment.

There is limited data available for the production processes of perovskite solar cell. As for most new emerging technologies, one dominant design in not established yet. Several variations of the cell exist depending on perovskite material used, material for hole transmitting material, and deposition method for the materials (Fan et al., 2014). In this study, one specific design was chosen since it is a relatively new design (2014), data is available, and the reported efficiency is close to the silicon solar cell described in section 2.3. Technical details of this design are presented in Table 5. Compared to the variations of material composition and production processes for perovskite solar cell (presented in Table 1 in the article by Fan et al., 2014), the design chosen in the study stands out from other designs in terms of the deposition method, where spin coating is assisted by vapour deposition process. In most of the other designs, spin coating is used for the deposition of both organic and inorganic parts of the cell (Fan et al., 2014). For most of the recent designs, Spiro-OMeTAD has proven to be the optimal hole transmitting material to achieve high efficiencies, and therefore this material is used in the study. Note that there are some variants of perovskite solar cell compositions that do not contain lead. However, in this study, in order to investigate the negative effects of lead content in solar cells, a perovskite material containing lead content was chosen.

Table 5. Material composition and performance summary of the studied perovskite cell. Part of Table 1 from Fan et al. (2014).

Perovskite material	Photoanode	Deposition method	Hole transmitting material	Area (cm^2)	Efficiency
$CH_3NH_3PbI_3$	TiO_2 (thin film)	Spin coating and vapour deposition	Spiro-OMeTAD	0.12	12.1%

Process data is collected from a research article published by Chen et al. (2014), in which a spin-coated, vapour-assisted process was used for material deposition. Blade coating technology, described by Hösel (2014), for layer deposition was also investigated in this study. It has to be noted that currently, there is only a small scale perovskite solar cell production and the up-scaling of these processes for large scale solar cell production is done only theoretically for the purpose of this study. In the future, for large-scale production of perovskite solar cells, these processes and material inputs could change due to the continuous research that is ongoing to develop the production of these cells.

Because of the lack of reliable data, some of the materials in the production process are excluded from the study. These material have only a minor part in production, and their impact, even in up-scaled production process, should be relatively low. These materials

are mostly various chemicals included in production of solar cell components, such as some gases used in chemical processes (argon, nitrogen) or liquid chemicals (hydrogen, ammonia) with low total mass input to the processes. Material inputs considered for the production of one perovskite solar cell are presented in Table 6.

Table 6.   Material inputs for the production of one perovskite solar cell.

Material:	Mass (g)
Indium tin oxide coated glass	0.17
Titanium dioxide	0.0005
Perovskite	0.4
Hole transport layer	0.013
Back contact	0.005

5.1   Initial flowchart for the process

Figure 10 shows the process flow chart for the production of perovskite solar cells. The production processes are described in more detail in subsequent sections.
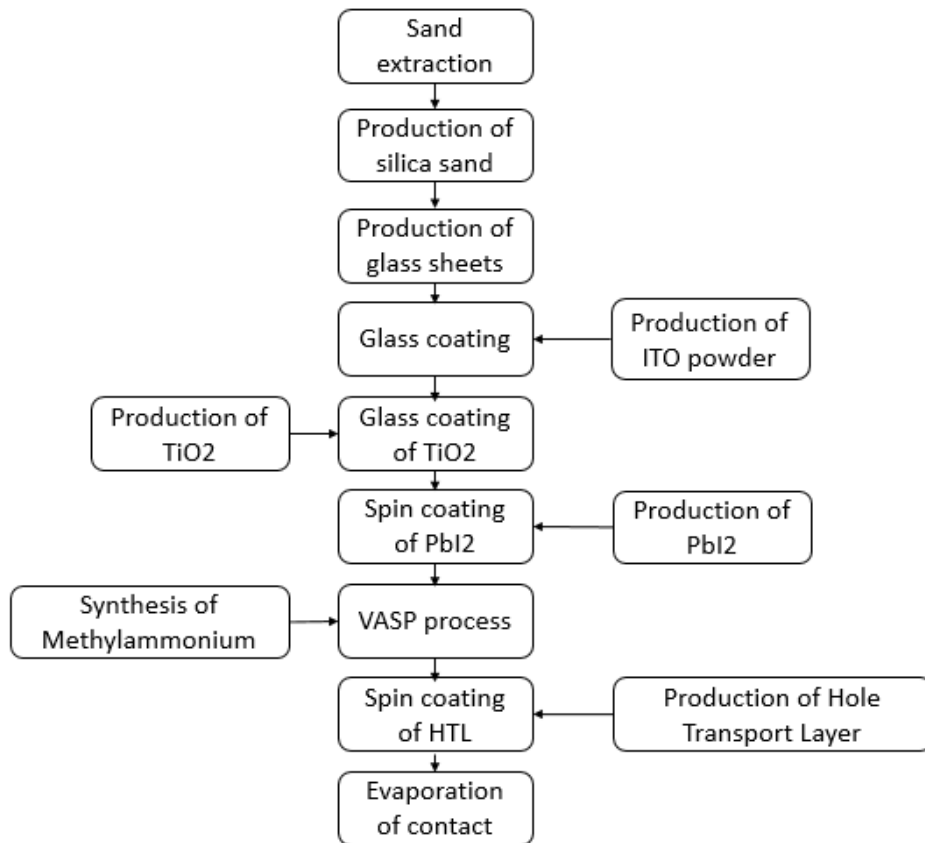
Figure 10.   Flowchart for production of perovskite solar cell. In the chart, ITO stands for indium tin oxide, TiO$_2$ for titanium dioxide, PbI$_2$ for lead (II) iodide, VASP for vapor-assisted solution process, and HTL for hole transport layer.

5.2   Indium tin oxide-coated glass

Glass coated with electric conducting indium tin oxide film is used in this study (Chen et al., 2014). As shown in Table 5, the total area of a perovskite cell is 0.12 cm^2. From this, we get the dimensions of required glass for one cell of about 3.5x3.5 mm. Data for the production of glass sheet is available in the Ecoinvent database as production of "flat glass, uncoated, at plant" (#806). Production data for indium tin oxide is also available in Ecoinvent database as "ITO powder, for target production, at plant" (#10142). There is a lack of data for the coating process of glass with indium tin oxide. For this, the process "anti-reflex – coating, etching, solar glass" (#803) process data has been chosen since the process is similar, and the only main difference is the input material for the coating of the glass.

5.3   Titanium dioxide

Indium tin oxide-coated glass is covered by a thin titanium dioxide layer using electricity and heat as energy inputs (Chen et al., 2014). Electricity and heat energy inputs are summarized and discussed later in the Section 5.7. In this process, several compounds are prepared and used separately and then mixed together using different processes to form a titanium dioxide layer on the indium tin oxide-coated glass (Chen et al., 2014). Due to lack of production data for these separate materials, an already premixed titanium dioxide named "titanium dioxide, production mix, at plant" (#3550) in the Ecoinvent database is used in this study.

5.4   Perovskite layer

The perovskite layer consists of two materials – methylammonium iodide (CH$_3$NH$_3$I) and lead (II) iodide (PbI$_2$) mixed together to form crystals. There are several technologies to achieve this perovskite layer. One of the proposed technologies is to premix the two main materials in a solution and to form a layer of perovskite (Fan et al., 2014). But it was found out that this method results in an incomplete surface coverage, which then results in lower performance of the cell and lower total efficiency (Fan et al., 2014). Another proposed process by Fan et al. (2014) is to use spin coating to cover the surface with lead iodide, and then to dip the film into an organic salt solution.

During the spin coating with vapour assisted deposition, lead (II) iodide is deposited on the film's surface using the spin coating technology, and the methylamine is then sprayed onto film via vapour assisted solution process (Chen et al., 2014).

The spin coating process is used to apply thin films onto materials (Brewer Science, 2010). Typical spin coating procedure includes applying a small amount of fluid onto the centre of a substrate, and then spin the substrate to make the fluid spread equally over the surface of substrate (Figure 11). Note that this process is used for obtaining relatively small and thin films and for production of these cells on a large scale, a

modified process or completely other process may be required. But considering a prospective nature of this study and the lack of data for large scale production of perovskite cells, this process with its energy and material use is investigated as one scenario in this study.
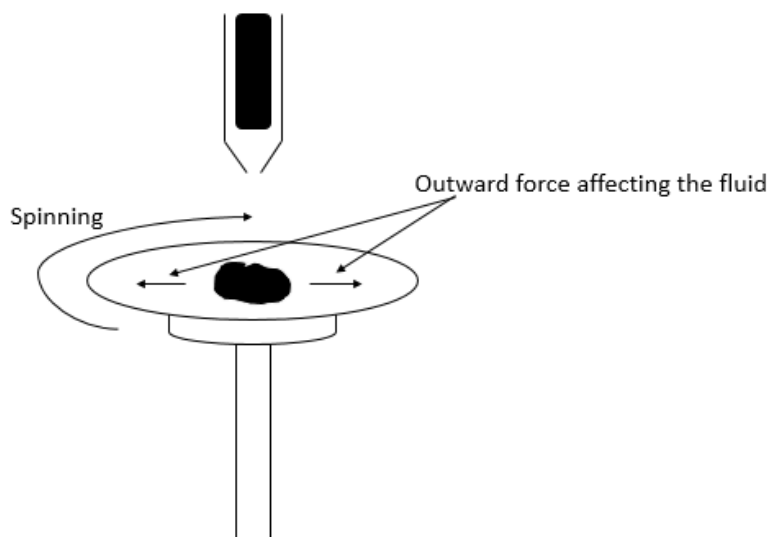
Figure 11.   Principle of spin coating process. Figure modified from Brewer Science (2010).

Recently, an alternative process to spin coating has been found, which more suitable for large-scale production. This process is blade coating. Because of the outward force that is affecting the material, most of the input material is typically lost during spin coating process, and only the remaining fraction is used for further cell production (Hösel, 2014). For this reason, the spin coating process is not suitable if perovskite cells should be produced on a larger scale. For large scale film production with blade coating, the blade is positioned over the moving film and the ink is applied over the blade in the small gap between the blade and the substrate to form a film (Hösel, 2014). The working principle of this process is show in Figure 12. For the purpose of this study, both the spin coating and blade coating processes are investigated.
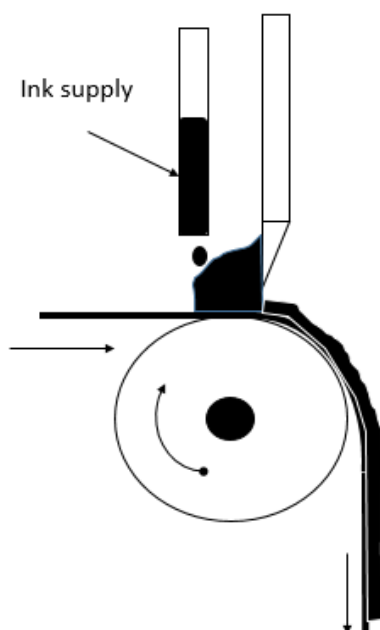
Figure 12.   Principle of blade coating process. Figure modified from Hösel (2014).

Vapor-assisted solution deposition process gives several advantages compared to spin coating and dipping, or depositing already premixed solution over the thin film (Fan et al., 2014):

- Lower temperatures are required for the process, which results in lower energy demands for the production

- Full coverage of the surface and low roughness of the surface. This leads to a higher performance of the cell and an increased overall efficiency

- Thermodynamic stability of the perovskite crystals over the growth process, yielding good grain structure.

Lead (II) iodide (PbI$_2$) is acquired directly from the producer as described by Chen et al. (2014). For this study, there was no data found for the production of this material and the material had to be decomposed into main elements with respect to available data in the Ecoinvent database. The main reaction to produce PbI$_2$ is as given below (Clark, 2004):

$$Pb(NO_3)_2 + 2KI \rightarrow PbI_2 + 2KNO_3$$
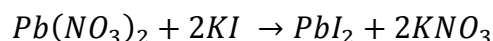
Data for potassium iodide (KI) was obtained from Ecoinvent (#50). Lead (II) nitrate (Pb(NO$_3$)$_2$) had to be decomposed further in order to obtain data for the production of materials (Clark, 2004):

$$Pb + 2NO_3 \rightarrow Pb(NO_3)_2$$
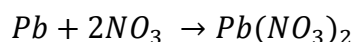
Lead (Pb) and nitric acid (NO_3) were found available in the Ecoinvent database as "Lead, at regional storage" (#1103) and "Nitric acid, 50% in H2O, at plant" (#299) respectively.

Methylammonium iodide is produced via the reaction described by Chen et al (2014): 24 mL of methylamine and 10 mL of hydroiodic acid are mixed in a round flask for two hours. Data for the components were found in the Ecoinvent database as "Methylamine, at plant" (#11250). Because of no data in the Ecoinvent database, a similar process regarding material and energy use was chosen instead of hydroiodic acid: "Hydrochloric acid, 36% in H$_2$O" (#6249). To account for the masses that are used in the reactions, stoichiometry calculations based on molar masses were used to account for the amount of hydrochloric acid that would be used instead of hydroiodic acid. The reaction as described by Chen et al (2014) looks as follows:

$$CH_3NH_2 + HI \rightarrow CH_3NH_3I$$

The resulting product was dissolved in ethanol (#6627) with a mixture of diethyl ether (#6623), and after drying in the vacuum, the mixture is ready to be spread over the film via vapor deposition process, as described by Chen et al (2014).

There are several suggestions for the mass ratio of the lead iodide and methylammonium iodide parts of perovskite film (1:1, 1:3, 1:4) (Chen et al., 2014), but for this study, a molar mass ratio of 1:1 was chosen.

5.5   Hole transport layer

The hole transport material (Spiro-OMeTAD) is deposited onto the perovskite layer using the same spin coating technology as for lead iodide (Chen et al., 2014). Main materials used here are 9 mg of chlorobenzene and 3.4 mg of acetonitrile to form hole transport layer (Chen et al., 2014). Required components were available in the Ecoinvent database as "Monochlorobenzene, at plant" (#6650) and "Acetonitrile, at plant" (#6613). According to Fan et al. (2014), most of the recent high-efficiency perovskite solar cells use this material as hole transport layer to achieve an as high efficiency as possible.

5.6   Back contact

As the final layer, a silver back contact is added using thermal evaporation technique. In the Ecoinvent database, the process named "Silver, at regional storage" (#10153) is chosen as a process for silver production.

5.7   Energy use

For the deposition of each layer of the cell, different sources and amounts of energy are required. In this study, the two main types of energy used in these processes are taken into account: electricity used in the spin coating processes and heat used during drying and heating. By knowing the exact power rating of the spin coating equipment and the source of the heating supply (which for this study is assumed by the average heating supply of the region), the electricity and heat requirement can be calculated (Table 7).

Table 7.   *Energy use for different processes in perovskite solar cell production (Chen et al., 2014).*

Layer deposition	Process	Energy/temperature	Time
Titanium dioxide	Spin coating	3000 r.p.m.	30 sec
	Drying	125°C	10 min
	Heating	550 °C	15 min
	Heating	550 °C	30 min
Methylammonium iodide	Drying	60 °C	24 hours
Lead (II) iodide	Spin coating	2000 r.p.m.	30 sec
	Drying	110 °C	15 min
Hole transport layer	Spin coating	2000 r.p.m.	30 sec
Silver back contact	Thermal evaporation	100 °C	10 min

To account for energy used in the processes, electricity and heating demand has been calculated for each process in Table 7. To account for the heating demand, where temperature is increased from an ambient to a desired temperature, the required energy is calculated using the following heat equation:

$$Q = C_p \times m \times \Delta T$$

where Q stands for the energy required in the process (J), C_p stands for the specific heat capacity of the material heated (J/kg·K), m stands for the mass of material heated in the process (kg) and ΔT stands for temperature difference (K or °C). For the processes where temperature levels have to be maintained for an amount of time, the energy requirements depend on the equipment that is being used. For this study, Thermo Scientific® Barnstead Large Oval Chamber Muffle Furnace has been chosen because it satisfies the required temperature levels of the processes (Spectrum, 2015). The required energy for these processes is calculated using the electrical power of the specified device as described by the manufacturer, and the time during which the specific temperature is maintained for each of the processes (Spectrum, 2015).

$$Q = P \times t$$

where Q stands for energy required for temperature maintenance (kWh), P for the electrical effect of the oven (W), and t for the time required to maintain the temperature (h). The electrical effect of the oven is 1488 W (Spectrum, 2015). Since the temperatures maintained are relatively low, the oven is not required to run on its highest electrical effect. For these calculation, half of the oven heating capacity is used: 744 W.

Table 8. Energy use for the process in perovskite solar cell production route.

Material	Mass (kg)	Specific heat capacity (J/kg·K)	Temperature range (K)	Time (h)	Energy (Wh)
Titanium dioxide	0.035	690	From 273 to 398	0.16	2.7
	0.035	690	Constant at 398	0.75	110
Methylammonium iodide	173	-	Constant at 333	24	3600
Lead (II) iodide	415	-	Constant at 383	0.25	370
Silver contact	0.035	-	Constant at 373	0.16	240

Because the requirement of electricity for the spin coating or blade coating processes is only a minor part when compared to the whole life cycle route (around 1% of the total electricity demand for the production of the solar cell), it can be neglected from the LCA. The only difference that will be taken into account, when comparing the two perovskite production processes is thus the differences in amount of material inputs.

5.8   Transport

Same as for the silicon solar cell production, considering that this is a prospective study, exact production locations and transport distances cannot be known. Indeed, this is particularly true for the perovskite solar cells. To make this comparison of the two solar cells as general as possible, the transport impacts for the perovskite solar cells are assumed to be exactly the same as for the silicon solar cell (see section 4.9). Emissions from the transportation are still included even though they are the same for the two products, in order to see if these emissions and energy use have a notable impact on the final results.

5.9   Electricity

In a same way as for silicon cell, electricity production for perovskite cell is generalized and varied in the sensitivity analysis. This is done in order to compare the two technologies on a general level, not for very specific situations that may or may not occur.

6   Impact assessment

This chapter demonstrates findings from the study and the sensitivity of different parameters is assessed.

6.1   Sensitivity analysis

In order to compare the two solar cells thoroughly and transparently, the variation of several parameters has to be considered. These parameters that are varied should have a notable effect on the amount of emissions released or the energy used of the production of solar cells. Because of the relatively low impact of the total emissions from transportation (1.5-3% for toxicity and energy use, for both toxicity assessment methods), transportation is not selected as one of the varied parameters. The parameters that are varied for the sensitivity analysis are instead the ones presented below:

- **Lead source for the production of perovskite solar cells.** Since lead is one of the main components for perovskite solar cells and one of the main topics of this study, it is important to consider different options for obtaining this material. Three different scenarios regarding lead origin are investigated in this study. The first is that all of the lead required for the production of perovskite solar cells comes directly from mining, meaning that the lead is pristine. The second is that all of the lead required for the production comes from recycling. The third is that half of the lead comes from mining processes and the other half from recycling. This parameter can be varied using data from the Ecoinvent database. The process "Lead, primary, at plant" (#10777) describes energy use and emissions from the production of lead with sinter/blast furnace and direct smelting process. This process uses lead concentrates that originates from mining. For the second scenario, the data set "Lead, secondary, from electronic scrap and recycling, at plant" (#8138) is used. This option represents a best case scenario where all of the lead comes from recycling. If considering large-scale production possibilities for the perovskite solar cells in the future, recycling as a way of obtaining lead for the production, could be a too small a source, considering different recycling rates in different regions of the world. The third scenario combines the two previous sources of lead in a 1:1 mass ratio, meaning that half of the lead comes from mining and the other half originates from recycling.

- **Electricity production mix.** For this study, three scenarios of electricity production mix were investigated in order to see how emissions from different energy sources would influence the final results. In one scenario, all of the electricity required for the production of both cells is supplied from coal-fired power plants (representing high-emission electricity production in general). In another scenario, half of the total electricity is supplied form coal-fired power plants and the other half is produced in natural gas power plants (roughly representing current central European electricity production). In a third scenario, half of electricity is produced from nuclear power plants and the other half coming from hydropower plants (roughly representing current electricity production in Sweden, but also low-emission electricity production in general).

- **Film production process.** For this parameter, two scenarios are investigated. The first is production of perovskite solar cells using only spin coating for the deposition of film layers. The second is production of perovskite cells using blade coating to deploy the film layers. The main consideration here is the use of materials, where blade coating technology is more applicable for large scale production since it has a lower material input. While the energy use is neglected for these processes (see section 5.7 for motivation), the considerable difference in amount of material input between the two processes has a large influence on the impact of the perovskite life cycle. For this parameter, using spin coating represents a worst case scenario and using blade coating represents a best case scenario.

- **Lead loss emissions.** For this parameter, loss of lead to the environment during two processes is considered. Several variations of this parameter are taken into account. For one case, there is no lead emitted during the production of perovskite solar cells, and no lead emitted during the use and recycling. Another case investigates a scenario where all of the lead lost during production process is emitted to the environment. Finally, in a third case, all of the lead that is contained in perovskite solar cells is emitted to the environment (during the use phase and/or recycling). This parameter should emphasize in which process it is extra important to manage the loss of lead and avoid emissions to the environment.

In this study, the parameters were varied in the following order: First, a possible future best case scenario was created as a baseline scenario. This case includes the Swedish electricity mix (half hydro and half nuclear), blade coating technology as the film deposition process, the entire supply of lead for the production of perovskite cells comes from recycling, and no lead loss emissions throughout the entire life cycle (neither during production nor in the use phase and/or recycling). This case is referred to as "best" in the following graphs.

Energy production parameters are changed next. "Gas/coal" represents half of the electricity from coal and half from natural gas for both studied cells. The case "coal" represents electricity production mix based entirely on coal-fired power plants.

This is followed up by changing the lead sources for the production of perovskite solar cells. The case where half of lead is supplied from mining and the other half is supplied from recycling is referred to as "50/50 lead recycled/mining" in the graphs. After this, all of the lead from recycling is removed, and the supply of this material is considered to be only from mining process, and referred to as "Lead mined".

Next, the lead loss emissions are investigated. The case where all lead waste during the production of solar cell is emitted to the environment, is presented as "lead production loss". And the other case, where all lead contained in the solar cell is emitted to the environment either during the use phase or during recycling, is presented as "lead content lost".

Finally, the film deposition technology was changed from blade coating technology to spin coating technology to represent energy use and emission differences between the two processes. This is referred to as "Spin coating" in the following graphs.

6.2   Ecotoxicity

Comparative results for ecotoxicity potential with different parameters varied are presented in the Figure 13. It can be seen that for the silicon cell results differ only when the electricity production mix is varied, since it is the only parameter that influences the results for this cell. For the perovskite solar cell, lead supply source and lead leakage from the cell has the largest influence on the results. While blade coating technology is a more material-preserving method for film deposition, the lead losses during the production process are low (only about 10%) as reported by Hösel (2014), thus giving low emissions for the lead production loss case.
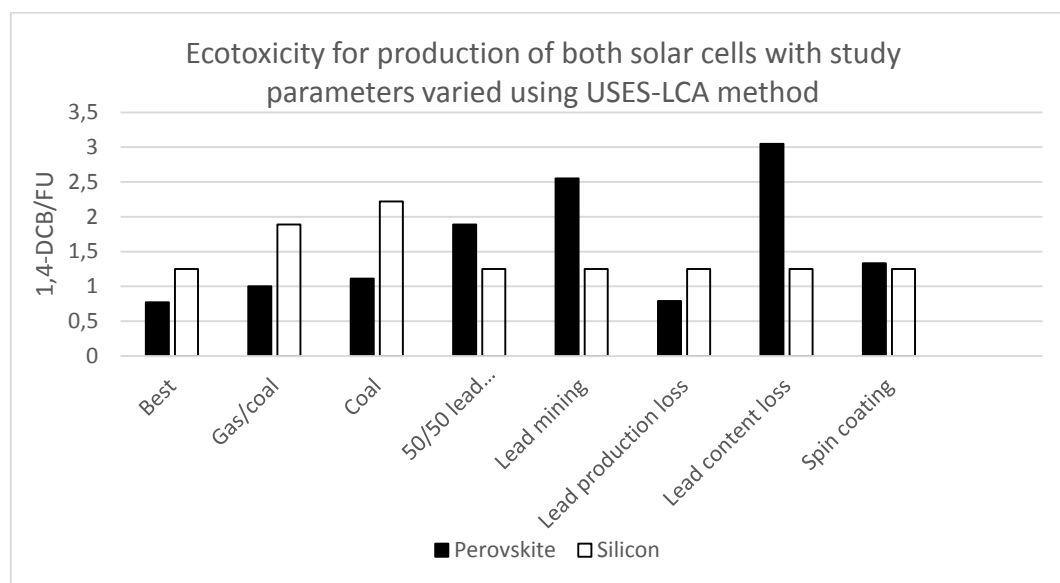
Figure 13.   Comparative results of ecotoxicity potential for production of 1 kWh of perovskite and silicon solar cells, using USES-LCA impact assessment method.

One of the largest influences regarding emissions for perovskite cells comes from lead mining processes. In the life cycle inventory, emissions contributing the ecotoxicity potential can be traced back and seen that cadmium and copper are the two main contributors to this category. Because of high amount of these heavy metals emitted during lead extraction, and high toxicity potential of these emissions, by reducing the amount of lead obtained from mining, lower ecotoxicity potential can be achieved. Changing the electricity production mix, and the amount of material input in terms of switching to spin coating, seems to have only minor influences to this impact category. This is mainly because these changes do not primarily influence the ecotoxicity potential. As can be seen from these results, it can be recommended to use lead from recycling processes for perovskite solar cell production, and to make sure that the lead contained within the perovskite cell is not emitted during use or recycling.

Emissions that contribute to ecotoxicity for silicon cell can be seen in Figure 14, and emissions that contribute to ecotoxicity for perovskite cell can be seen in Figure 15.
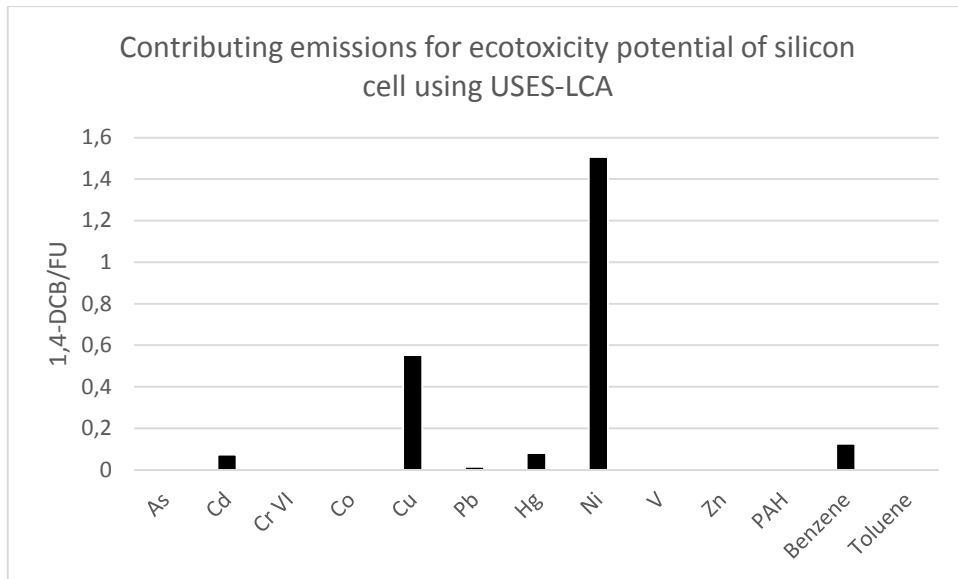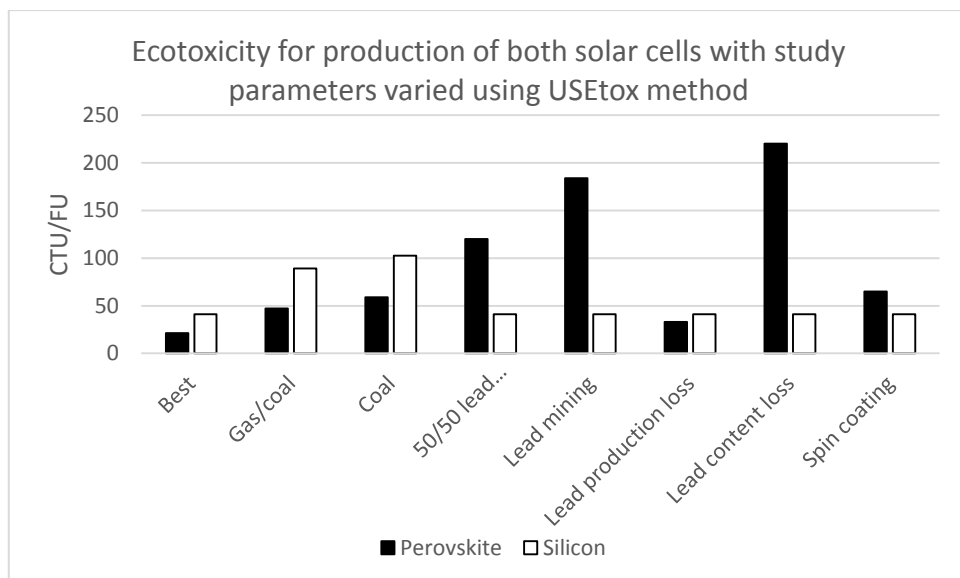
Figure 14.   Emissions that contribute to ecotoxicity for silicon solar cell using the USES-LCA impact assessment method for the best case scenario.
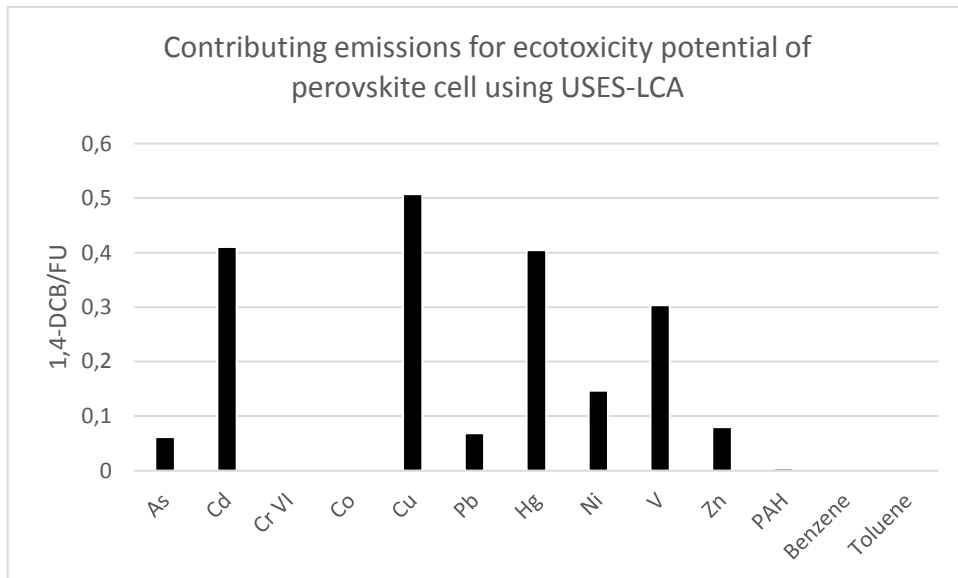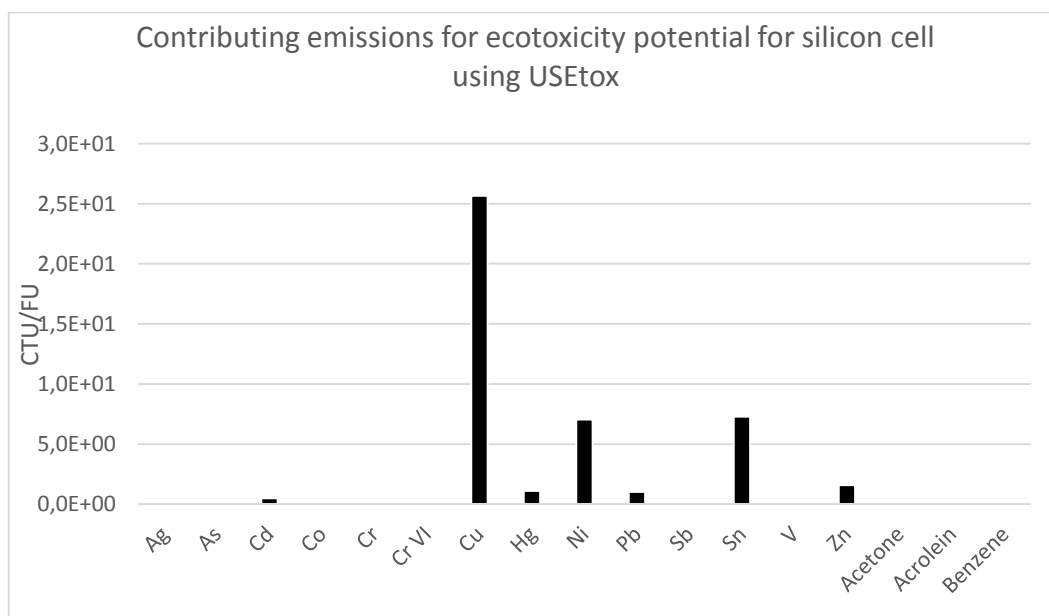

Figure 15.   Emissions that contribute to ecotoxicity for perovskite solar cell using the USES-LCA impact assessment method for the best case scenario.

Using the USEtox method for toxicity impact assessment gives results that emphasize emissions from lead mining even more, as can be seen in Figure 16. This can be seen from the case where half of lead to the production process of perovskite cell is supplied from recycling. Notably, regardless of which impact assessment method is used, the crucial parameters for the perovskite cell are the same, emphasizing the importance of lead supply source and the importance of maintaining the lead in a cell during the use and recycling phases of a cell's life cycle.

Figure 16. *Comparative results of ecotoxicity potential for production of 1 kWh from perovskite and silicon solar cells for all scenarios, using the USEtox impact assessment method.*

Emissions that contribute mostly to ecotoxicity potential using the USEtox impact assessment for silicon and perovskite solar cells are presented in Figures 17 and 18, respectively. As can be seen from the figures, some of the major contributors are the same regardless of which impact assessment method is used. For both methods, copper and nickel contribute much for the silicon cell, and copper contributes much for the perovskite cell.

Figure 17. *Emissions that contribute to ecotoxicity for silicon solar cell using USEtox impact assessment method.*
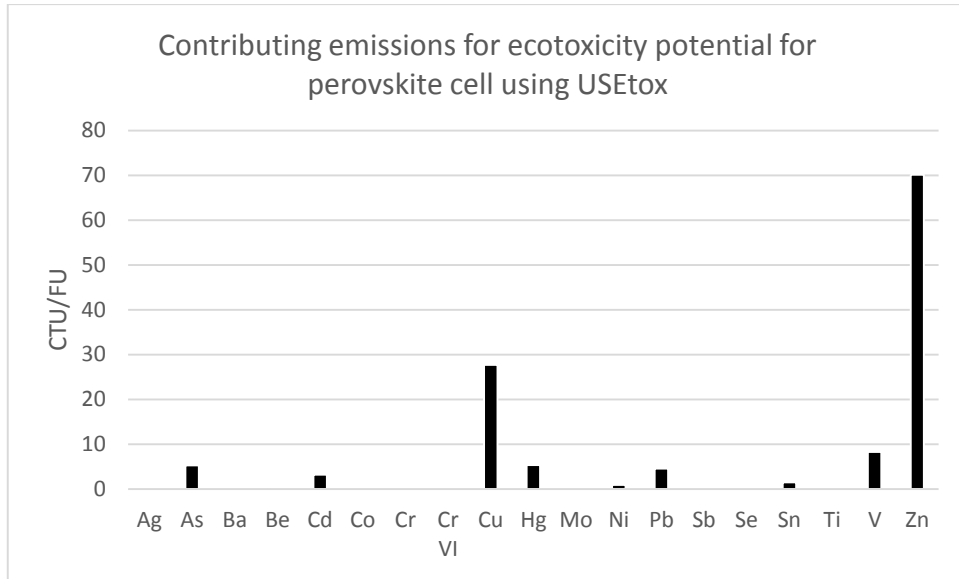
38

Figure 18.   Emissions that contribute to the ecotoxicity of the perovskite solar cell using the USEtox impact assessment method for the best case scenario.

6.3   Human toxicity potential

Comparative results for human toxicity potential for different scenarios are presented in Figure 19. As seen from Figure 19, there are major differences for different scenarios for the perovskite cell. Major contributors to this category can be traced back in life cycle inventory and identified as arsenic and cadmium for perovskite solar cells. As for the ecotoxicity impact category, most of these emissions come from lead mining process. That is why changing the ratio of lead supplied by recycling has a major influence on the final results. And because of higher characterization factors of arsenic and cadmium for human toxicity than for ecotoxicity, these emissions have a more profound contribution here.
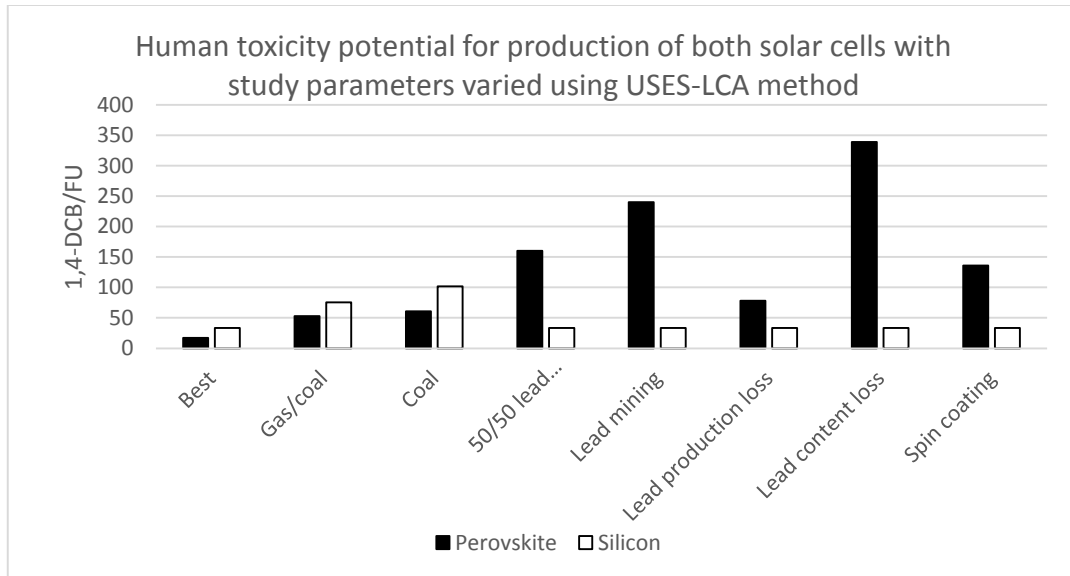

Figure 19.   Comparative results of human toxicity potential for production of 1 kWh from perovskite and silicon solar cells using the USES-LCA impact assessment method

For silicon solar cells, the human toxicity potential increases slightly when the electricity production mix is varied. As expected, the electricity mix based on hydropower and nuclear gives the best results for this cell. For other parameters, the impact does not change for silicon cell, because the parameters do not influence production of this cell. For perovskite solar cells in Figure 19, similarly to the ecotoxicity, the results change considerably when the lead supply is varied. It has to be noted that human toxicity category has more emphasis on the lead loss scenarios, where lead emitted from the solar cell itself or its production would result in a notable increase in human toxicity potential.

Emissions contributing to human toxicity potential for silicon solar cell are presented in Figure 20. Emissions contributing to human toxicity potential for production of perovskite solar cells are presented in Figure 21. Main emissions here are arsenic and cadmium, which originate from lead mining.
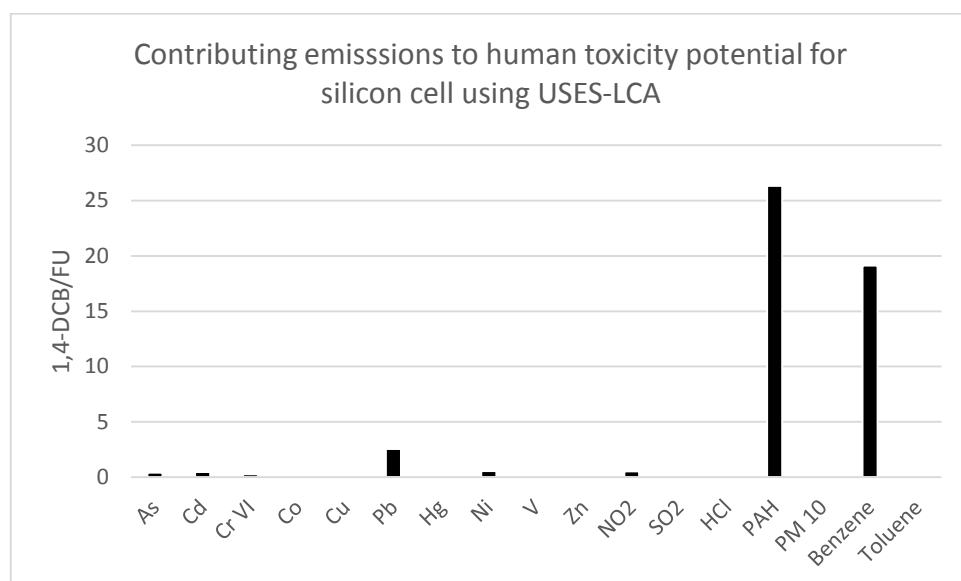

Figure 20.   Contributing emissions to the human toxicity potential for silicon solar cells using the USES-LCA impact assessment method for the best case scenario.
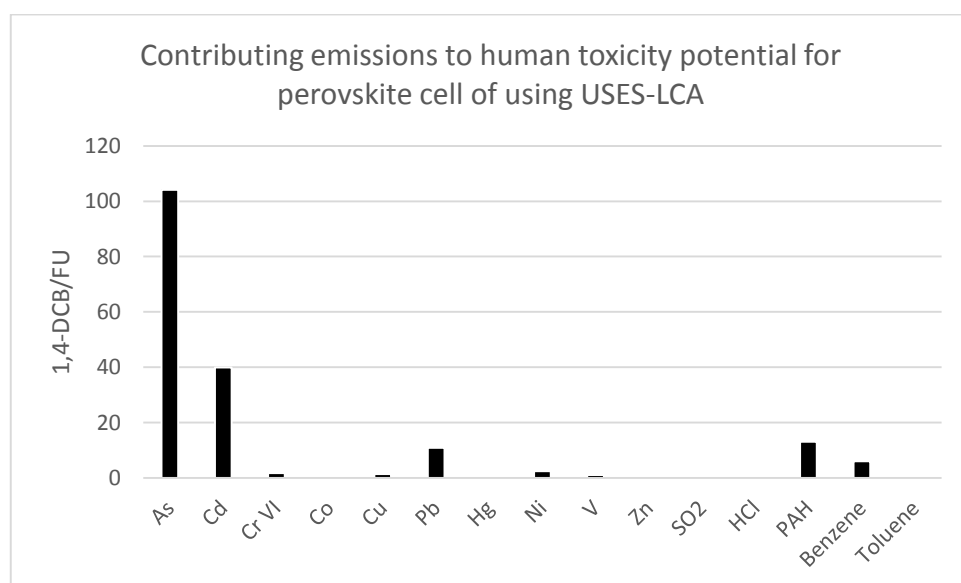

Figure 21.   Contributing emissions to the human toxicity potential for perovskite solar cells using the USES-LCA impact assessment method for the best case scenario.

40

Results for human toxicity potential for all cases using the USEtox impact assessment method are presented in Figure 22. From the results, it can be seen that the USEtox method emphasizes lead as an emission more compared to the USES-LCA method. This shows the importance of choice of impact assessment method for LCA studies. In order to present results for this category and impact assessment method more clearly, the lead content loss case is removed and the other scenarios are shown in Figure 23. The lead content loss case was removed since it is the dominating emission in Figure 22, which makes it hard to see the other contributions.
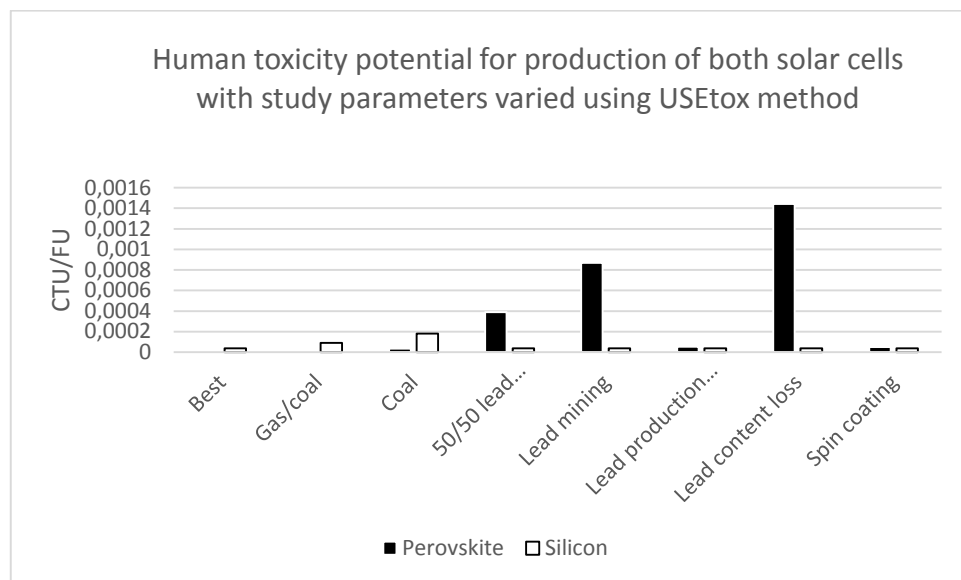
Figure 22.   Comparative results of human toxicity potential for production of 1 kWh from perovskite and silicon solar cells, using the USEtox impact assessment method.
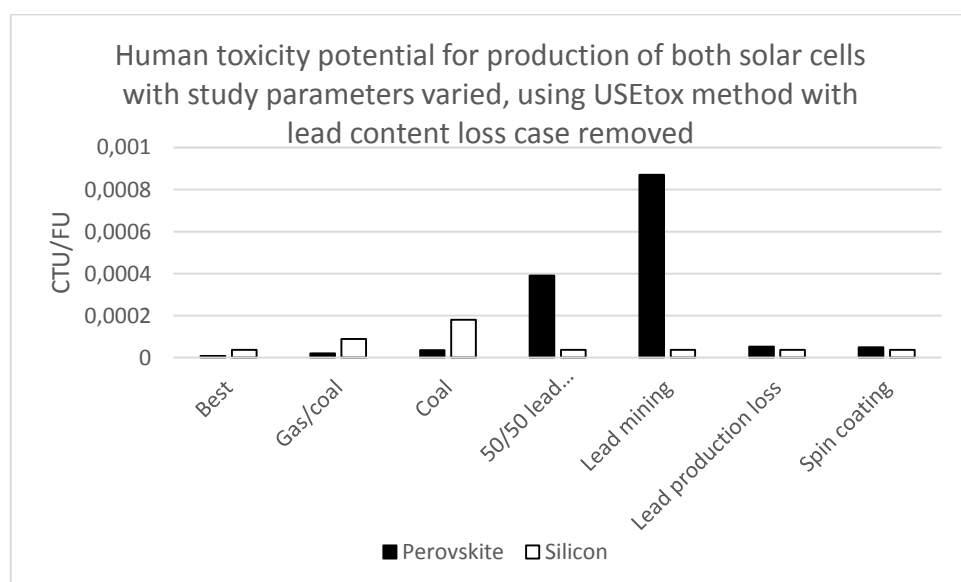
Figure 23.   Comparative results of human toxicity potential for production of 1 kWh from perovskite and silicon solar cells, using the USEtox impact assessment method, with lead content case removed.

Now, similarities between two impact assessment methods can be identified. Lead is indeed a main issue here, but for best case, and all electricity mix scenarios, the perovskite cell still gives better results compared to silicon cell.

When comparing the two impact assessment methods with respect to the largest contributors to human toxicity, it can be seen that the main contributors are similar between two impact assessment methods Contributing emissions to human toxicity potential for both cells, using the USEtox impact assessment method, are presented in Figures 24 and 25. Copper is the main contributor for the silicon cell, and lead for the perovskite cell.
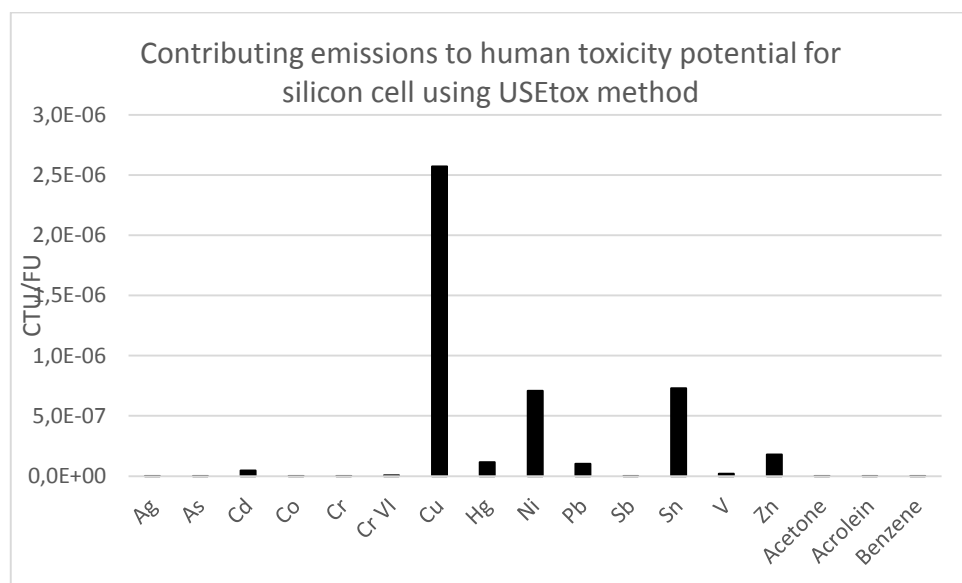

Figure 24.   Contributing emissions to human toxicity potential for the silicon solar cell using the USEtox impact assessment method for the best case scenario.
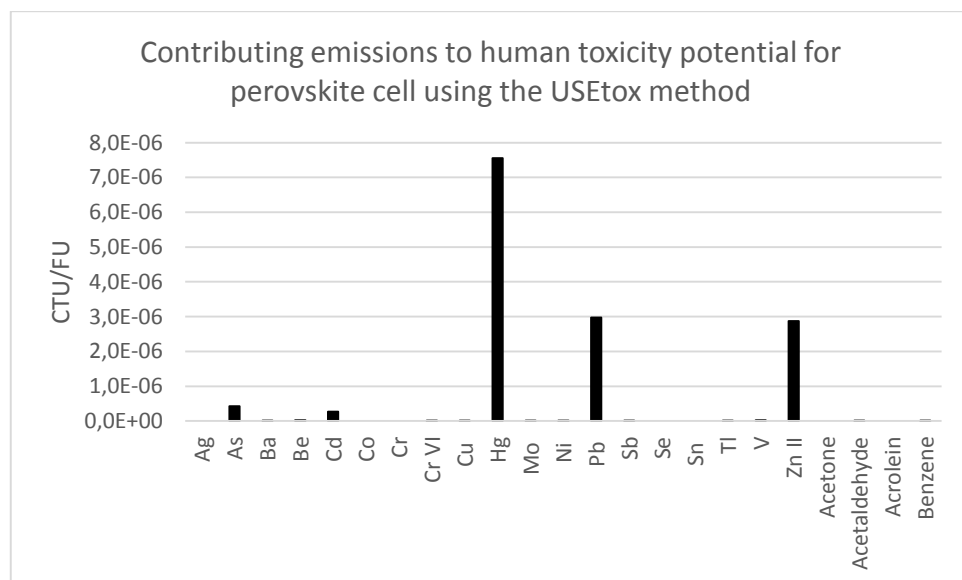

Figure 25.   Contributing emissions to human toxicity potential for the perovskite solar cell using the USEtox impact assessment method for the best case scenario.

6.4 Energy use

For this impact category, total energy demand is separated into thermal energy and electric energy. Demand for thermal energy for all cases is presented in Figure 26. Because there are no parameters that are changed in the sensitivity analysis that would affect the demand of heat or electricity for silicon solar cell, there are no changes in this energy use for this cell and thus the result for this cell is presented only once in Figure 26. For the perovskite cell, most of the heat energy is required for lead mining, and reducing the amount of lead from the mining in favor of recycled lead results in lower demand for thermal energy. Also, using the blade coating technology instead of spin coating results in lower material input and thus also in lower thermal energy demand
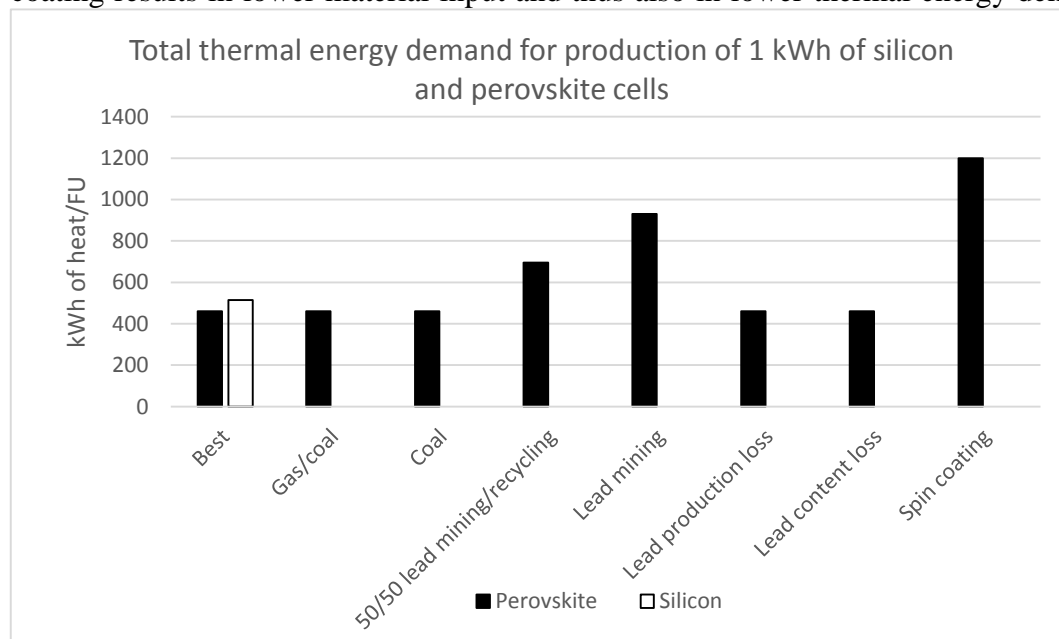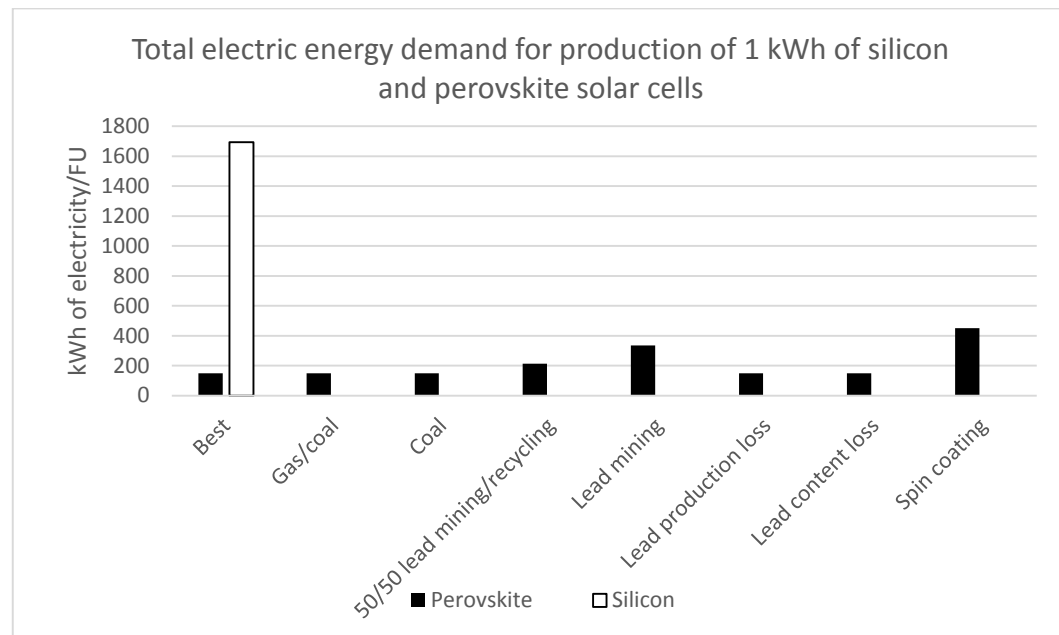

Figure 26. *Total thermal energy demand for production of silicon and perovskite solar cells, for all scenarios.*

It can be seen that for the best case and all electricity mix scenarios, the thermal energy demand for the perovskite cell is slightly lower than for the silicon cell, but increases largely when some other parameters are changed. This can be explained that for production of perovskite cells, mostly chemical processes where the demand for thermal energy is high are used, for example for mixing of the chemicals and maintaining temperatures at specific levels.

As for the thermal energy demand, there are no changes of electric energy demand for the silicon solar cell between scenarios, because no parameters that would influence that have been changed throughout the scenarios. Again, for the simplicity, the result for silicon solar cell is presented only once in Figure 27, and is the same throughout all scenarios. Electricity demand for both solar cells, and for all scenarios, is presented in Figure 27. As can be seen from Figure 27, the electric energy demand for silicon solar cells is higher than for perovskite solar cells for all scenarios. From the life cycle inventory, processes that are most energy intensive can be identified. Production of high purity solar grade silicon is the most energy demanding regarding electric energy. As mentioned in section 4.5, this process uses the modified Siemens technology, which is less energy demanding than usual Siemens process. Electric energy demand would be even higher if the older technology would be used for the production of silicon solar cells. For the perovskite solar cell, the most electricity-intensive process is production

of lead (II) iodide, where various chemical processes and lead mining require much electricity. However, by using different material deposition technologies (blade instead of spin coating), the required amount of material input can be reduced, and thus also the electric energy demand.

Figure 27.   Total electric energy demand for production of silicon and perovskite solar cells, for all scenarios.

7 Concluding discussion

This section summarizes findings of the study, giving a recommendation and answering the research question and thus fulfilling the purpose of the study.

The research question of this study was: "Which of the two solar cells has a lower impact on the environment throughout its life cycle?" The assessment conducted in the study showed that it is not so easy to answer this question without taken several aspects into consideration. Since the production of such complex technologies as solar cells are investigated in this study, several scenarios had to be considered in this study.

First, it should be noted that in the best case scenario, the perovskite solar cells had better toxicity and energy use performance then the silicon solar cells. This shows that the perovskite solar cells has the potential to have a better environmental performance than the silicon solar cells. However, a number of conditions must be fulfilled for this best case to become realized, as was shown in the sensitivity analysis of this study.

It was found out that the production of primary lead for the production of perovskite solar cells had a large influence on the final results. For both the ecotoxicity and human toxicity impact categories, silicon solar cells have lower impacts when all of the lead is obtained from mining processes. But for the scenario where all of the lead is supplied from recycling, the perovskite cells show better results than the silicon cells. This is true no matter which of the two toxicity impact assessment methods are used: USES-LCA or USEtox. The electricity production mix was taken into account in the study, but had only minor influence on the results. One of the other changed parameters in the study was the manufacturing technology for perovskite solar cells. Both spin coating and blade coating technologies were assessed. The study showed that blade coating technology is the preferred option here, with lower material requirement and emissions from the production.

An additional parameter that was changed was losses of lead from production, use and disposal processes of the perovskite solar cell. From the results, it was seen that emissions of lead during production, use or recycling could cause the perovskite solar cell to have higher toxicity impact than the silicon solar cell. Particularly emissions of the lead contained within the cell during the use phase and recycling should be avoided if considerable toxicity impacts are to be avoided.

Notably, although the results from the two toxicity impact assessment methods generally provided the same main messages, the details of the results were not always similar. For example, the two impact assessment methods did not always show the same main contributing emissions. This emphasizes the importance of including several toxicity impact assessment methods to test the robustness of the results.

From the energy demand perspective, it was found that different types of energy are used for the two solar cells. Silicon solar cell use mainly electric energy in its production chain, and perovskite cells require mainly energy in the form of heat.

It is interesting to compare the use of lead in perovskite solar cell with other technologies that have lead content in their production. The automobile industry uses around 1 million tonnes of lead every year. And even if recycling of lead-acid batteries is considered one of the most successfully implemented recycling programs, over 40 thousand tonnes of lead end up in landfills every year (Battery Council International, 2012). With the same amount of lead that is used in the automobile industry every year, around 25 GWh of perovskite solar cells could be manufactured, which approximately

equals the total electricity production from solar cells globally in the year 2009 (IEA, 2012). If this same amount, 1 million tonnes of lead, would indeed be used for production of solar cells, over 60 thousand tonnes of lead would be wasted from production (although not necessarily emitted), provided that the more efficient blade coating technology was used. This is slightly higher than the 40 thousand tonnes for car batteries. However, since recycling of car batteries is considered a successful recycling program with low amounts of waste, it could be that similarly successful recycling schemes could be implemented for perovskite solar cells, hopefully creating closed loop systems with no net waste of lead.

In conclusion, it can be said that perovskite solar cells have potential to rival the curently dominating silicon solar cells from an environmental perspective. If to be produced on a large scale, and this better environmental performance is to be realized, there are two main issues to consider: (1) the supply of lead should preferably be from recycled lead, and (2) emissions of lead from the perovskite solar cells itself should be avoided.

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