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Grado en Ingeniería de Organización Industrial

Análisis de los materiales utilizados en la producción de células solares con las tecnologías actuales y las prometedoras: un enfoque con la Dinámica de Sistemas.

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- TÍTULO: Analysis of the materials used in solar cells production with the current and the promising technologies: a System Dynamics approach
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SECCIÓN I:

RESUMEN EN CASTELLANO Y EN INGLÉS



UNIVERSIDAD DE VALLADOLID

RESUMEN:

Las células solares más extendidas en el mercado fotovoltaico actual están principalmente compuestas de silicio, pero su procesado es relativamente caro debido a la alta pureza requerida para este material. Además, las tecnologías fotovoltaicas que emplean silicio se encuentran considerablemente estancadas en cuanto a mejoras en su eficiencia de conversión energética. En los últimos cinco años se ha investigado una nueva prometedora tecnología fotovoltaica con la que se podría obtener una eficiencia mucho mayor a unos costes de producción más bajos. El material revolucionario de las células solares desarrolladas por esta tecnología es la perovskita, cuyo principal compuesto es el plomo.

Mediante un modelo de Dinámica de Sistemas, este Trabajo Fin de Grado simula y analiza el consumo y reciclaje de los materiales empleados en las distintas tecnologías fotovoltaicas durante las próximas décadas, la evolución de su capacidad, y otras cuestiones que ponen en duda el uso de la perovskita.

Palabras clave: Células solares, Silicio, Perovskita, Plomo, Dinámica de Sistemas.

ABSTRACT:

The most common solar cells in the current photovoltaic market are mainly made by silicon, but their manufacture is relatively expensive due to the high purity required for this material. Moreover, the silicon based photovoltaic technologies are considerably stagnant in terms of improvements in their power conversion efficiency. In the last five years there was an important research about a new promising photovoltaic technology, which could reach much higher efficiencies with lower production costs. The revolutionary material for the solar cells developed by this technology is perovskite, whose main compound is lead.

Through a System Dynamics model, this Thesis simulates and analyzes the consumption and recycling of the materials used in the different photovoltaic technologies over the coming decades, the evolution of their capacity, and other issues that question the use of perovskite.

Keywords: Solar cells, Silicon, Perovskite, Lead, System Dynamics.

<u>SECCIÓN II:</u> MEMORIA EN INGLÉS



UNIVERSITY OF BERGEN

ANALYSIS OF THE MATERIALS USED IN SOLAR CELLS PRODUCTION WITH THE CURRENT AND THE PROMISING TECHNOLOGIES: A SYSTEM DYNAMICS APPROACH.

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ABSTRACT

In a world where its economies are currently driven by the fossil fuels, the need of renewable energy sources is becoming more and more urgent. Energy demand in society is constantly increasing while the resources of fossil fuels reduce. Solar energy seems to be the most attractive alternative for an inexhaustible energy supply. Photovoltaics (PV) is the main technique to produce electricity coming from sunlight and its price is becoming close to compete with fossil fuels.

The fast development of both the current and promising photovoltaic technologies carries several concerns that question the viability of a large scale solar capacity in the world. The global consumption of the materials required for solar cells production may rapidly increase with the growth of photovoltaics and problems of scarcity could appear. Therefore, recycling would become fundamental to be able to expand solar capacity in a sustainable way.

The future evolution of photovoltaic technologies and their used materials is analyzed in this study through a simulation model based on System Dynamics built to face these and others issues.



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1. INTRODUCTION

Fossil fuels have always been the main source of energy as they are able to produce significant amounts of energy. Petroleum, coal and natural gas are the major fossil fuels and current world's economies have a strongly dependence on them. Nevertheless, there are two big concerns: fossil fuels are finite resources and their use raises serious environmental worries.

Lot of energy alternatives have been developed in the last decades, including clean coal, nuclear and a long array of renewables like biomass, hydropower, geothermal, waves, wind and solar. However, all these options do not have the same capability. Maybe the researches should focus on the development of one of these alternatives instead of developing such a big mix.

Solar energy is the technology that makes useable the energy from the sun and it is the source with the biggest potential among all the energy sources. The sun power annually intercepted by the earth, only by the emerged continents and assuming losses of 65% by the atmosphere and the clouds, is around 23 000 TW (Perez et al., 2009, "A Fundamental Look at Energy Reserves for the Planet").



Figure 1. Global energy potential by sources. Source: Perez et al., 2009, "A Fundamental Look at Energy Reserves for the Planet".

Worldwide energy consumption was about 16 TW in 2009 and the International Energy Agency (IEA) estimates that it will be approximately 20 TW by 2035. If we compare these values of energy use with the global solar power we can assume that solar energy is a limitless resource. Moreover, it is consider a renewable source of energy since sunlight is naturally replenished on a human timescale.



There are different technologies to produce power coming from solar. These different techniques differ on the way they capture, distribute or convert solar energy. Photovoltaic systems, also called solar PV, are the most used and they employ solar panels composed by several solar cells.

When sunlight strikes the solar cell, its photons are absorbed by the semiconductor material and electrons are excited so that some of them leave their atomic orbital and reach an electrode. These current flows create the electricity that can be captured.



Figure 2. Operation of a basic solar cell. Source: NASA Science, 2002, "How do Photovoltaics Work?".

The problem is that photovoltaic energy is expensive compared with fossil fuels, but big improvements are being done in order to make solar energy competitive in price. Figure 3 shows how the cost of photovoltaic has decreased since 1990 and is now close to reach the average cost of fossil fuels.







While the cost of solar panels have been decreasing over time, the investments in photovoltaics have rapidly increase in such a way that the solar global capacity has experienced an exponential growth in the last decade.



Solar PV Total Global Capacity, 2004–2013

Figure 4. Solar PV total global capacity (2004-2013). Source: REN21, 2014, "Renewables 2014 Global Status Report".

Solar PV has been recognized as a promising renewable energy able to replace the fossil fuels. For this reason, lot of governments implemented several programs to encourage the use of this technology.

If improvements in solar cells continue reducing costs in the future, the investments in photovoltaics will keep evolving with the same tendency and the solar global capacity may be one day the main energy source in the world.

This paper is focused on both the current and future promising photovoltaic technologies. In the next chapter these technologies are presented and in the third chapter the identified problems and concerns are exposed. Then, it is explained the building of the model based on system dynamics that is used as method for this analysis, including the hypothesis made. Finally, this study analyses the results from the model and draws the conclusions.



2. SOLAR CELLS TECHNOLOGIES

2.1 Solar cells nowadays

2.1.1 The material: Silicon

The current PV market is dominated by silicon-based technologies, where silicon is the semiconductor material that absorbs sunlight.

After oxygen, silicon (Si) is the second most abundant element in the Earth's crust since 90% of it is composed of silicate material, according to the U.S. Geological Survey. It is also the eight most common element by mass in the entire universe. This material is widely found in the earth's surface in form of silicon dioxide, commonly known as sand, and its supply can be considered inexhaustible.

However, the silicon metal able to generate electricity that is used in photovoltaics is not coming from sand. The required silicon for solar cells manufacturing has to be highly pure (>99.9%) and it is technically called electronic grade silicon. This extremely pure silicon is derived from silicon metal, which is obtained after processing the minerals quartz or quartzite. The supply of these two minerals is also considered as inexhaustible by the U.S. Geological Survey.

Quartz and quartzite are formed by relatively pure crystalline silicon dioxide. The goal of their process is to chemically reduce the silicon dioxide into silicon metal, the precursor of the grade silicon. This process needs an expensive intense heat for melting, and the next purifying process to obtain the grade silicon involve also major costs.

Not all the different silicon solar cells need the same purity so their production cost may vary. The required purity level of the silicon wafers depends on the photovoltaic application.

Even if pure silicon is not precisely cheap, it is nowadays the most popular material in photovoltaics due to its very good properties. The most important property of silicon is that it produces electricity when sunlight strikes it. That happens because pure silicon is an intrinsic semiconductor so that it is able to conduct electrons and electron holes that are excited from the atoms by heat. So the most received solar energy, the most temperature and consequently the most electron movements, that is electricity.

Furthermore, silicon is not soluble in water and it is very resistant to high electrical powers and high temperatures.

Metals such as copper could not be used for this function in solar cells because, even if they have a very high conductivity, they cannot produce electricity.



Despite of producing electricity, pure silicon has a high resistivity so it is not a really good conductor. To increase its conductivity, pure silicon is doped in small proportions with other elements such as phosphorus and boron. In general, a solar cell has two layers of silicon with different electric charges. One layer is doped with phosphorus (n-type) and the second layer is doped with boron (p-type). So in Figure 5, the "p" and "n" represent the two doped layers of semiconductor silicon for the p-n junction.



Figure 5. Structure and mechanism of a basic silicon solar cell. Source: Wikipedia, "Solar Cell".

There are other raw materials which compose a basic silicon solar cell in smaller quantities. Silicon wafers are too shiny so they need an anti-reflective coating. The common materials for these anti-reflection layers are silicon dioxide (SiO2) or titanium dioxide (TiO2). Besides, solar cells are encapsulated into silicone rubber or ethylene-vinyl acetate (EVA) and then placed into an aluminum or steel frame and finally into a glass or plastic cover.

Electrical contacts, which connect each solar cell to another inside the solar panel and then to the receiver of the produced electricity, are usually made of metals such as silver-palladium (Ag-Pd), nickel (Ni) or copper (Cu). These contacts are really thin in order to do not block sunlight. In addition, between the cells of a solar panel there are placed thin strips commonly made of tin-coated copper. Solar panels also have an inverter to convert the variable direct current (DC) output into alternating current (AC).

The required quantities of all these other materials are considerably insignificant compared to the amounts of silicon needed for the semiconductor layers.



2.1.2 Types of silicon solar cells

Among all the silicon-based technologies, cells made of crystalline silicon (c-Si) are the most commercialized with a global market share of around 90% (Tatsuo Saga, 2010, "Advances in Crystalline Silicon Solar Cell Technology for Industrial Mass Production"), followed by thin-film solar cells.

Cells made of crystalline silicon, also known as solar grade silicon, are divided in two big categories: monocrystalline silicon (mono-Si) and polycrystalline silicon (multi-Si). The main difference between these two materials is about the crystallinity and the size of crystal. Other c-Si categories less present in the photovoltaic market are ribbon silicon and mono-like-multi silicon.

Monocrystalline silicon cells are more efficient than those made from polycrystalline silicon, as its silicon has a higher level of purity. However, multi-Si cells are more commonly used because they are less expensive. Figure 6 shows the global annual photovoltaic production by technology since 2000. It can be also observed the huge increase of PV production in the last decade.



Data: from 2000 to 2010: Navigant; from 2011: IHS (Mono-/Multi- proportion estimated). Graph: PSE AG 2014

Figure 6. Global Annual PV Production by Technology (2000-2013). Source: Fraunhofer ISE, 2014, "Photovoltaics Report".

Thin-film solar cells based in silicon usually use amorphous silicon (a-Si) as light-absorbing material and they are made by deposition of one or more thin layers on a substrate. In general, this type of cell has less efficiency than crystalline silicon cells but its production cost is cheaper. Some benefits of these cells are that they are lighter and more flexible, so that they are often used in building integrated photovoltaics replacing conventional building materials in the roof or facades.



2.1.3 Improvements in silicon solar cells

The main parameter to measure the performance of a solar cell is its efficiency, which means its power conversion efficiency (PCE). That PCE is the percentage of solar energy received by the cell that is converted into electricity.

There are some standard test conditions to measure the efficiency of terrestrial solar cells: an air mass 1.5 (AM_{1.5}) spectrum, an irradiance of 1000 W/m² and a temperature of 25°C.

The formula which gives the power conversion efficiency of a solar cell is:

$$PCE = \frac{P_m}{E \cdot A}$$

Where P_m is the cell's power output at its maximum power point (in watts), E is the input sunlight (in watts/m²) and A is the cell's surface area (in m²).

The first crystalline silicon solar cell was fabricated in 1953 at Bell Laboratories with a PCE of 4.5%. Over the next decade the efficiency was gradually improved to about 15% for these cells but, because of the high prices, the only significant applications were for spacecraft where the small weight of cells was a very interesting advantage. Prices were basically determined by the cost of the semiconductor material and as the space users were willing to pay big amounts for high-efficiency cells, there were no big inversions in research of low-cost and less-efficient technologies.



Figure 7. Evolution of solar cells efficiencies by technology. Source: NREL, 2013, "Best research solar cell efficiencies".



The basic crystalline solar cell structure that is currently used in industry was not developed until the 1970s, and the key technologies able to make solar cells to reach efficiencies higher than 20% were developed in the decades of the 1980s and 1990s. The most recent high-efficient silicon solar cells still have most of the properties of these technologies. The evolution of solar cells efficiencies by technology from 1975 to 2013 is shown in Figure 7. Note that, even if single-junction GaAs and multi-junction technologies have higher efficiencies than silicon solar cells, their prices are prohibitively expensive and that is why silicon cell dominate the current market. The efficiency improvements in silicon solar cells with a practical size since 1983 are presented in Table 1.

Table 1. Improvements in silicon solar cell efficiencies.Source: Martin A. Green, 2009, "The Path to 25% Silicon Solar Cell Efficiency: History of
Silicon Cell Evolution".

Date	Reported efficiency (%)	Test conditions*	Corrected efficiency (%)	Cell description
1/83	16.5	SERI 1 (t)	15.9	ORNL
5/83	17.1	SERI 1 (t)	16.5	ASEC
8/83	17.1	SERI 1 (ap)	16.5	Westinghouse
9/83	18.0	SERI 1 (t)	17.4	Spire textured
	18.7	SERI 1 (t)	18.1	UNSW MINP
12/83	19.1	SERI 1 (t)	18.4	UNSW PESC
5/85	19.8	SERI 1 (ap)	19.1	UNSW PESC
10/85	20-0	SERI 2 (ap)	20.2	UNSW µg PESC
7/86	20-6	SERI 2 (da)	20.8	UNSW µg PESC
4/88	21.4	SANDIA 2 (ap)	21.0	UNSW µg PESC
9/88	22.3	SERI 2 (ap)	22.5	Stanford
6/89	23-2	SANDIA 2 (ap)	22.6	UNSW PERC
12/89	23.0	SERI 2 (ap)	23.2	UNSW PERL
2/90	24-2	SANDIA 2 (ap)	23.4	UNSW PERL
3/94	23.5	ASTM E892 (ap)	23.7	UNSW PERL
9/94	24.0	ASTM E892 (ap)	24.2	UNSW PERL
2/98	24-4	ASTM E892 (da)	24.7	UNSW PERL
11/98	24-5	ASTM E892 (da)	24.7	UNSW PERL
3/99	24.7	ASTM E892 (da)	25.0	UNSW PERL

*(t) = total area, (ap) = aperture area, (da) = designated illumination area.

The last record efficiency for a crystalline silicon solar cell was 25% by a passivated emitter with rear locally diffused (PERL) cell and it was reported in the year 1999. Nevertheless, three important companies affirm to have broken this record in 2014. Panasonic's HIT solar cell is nowadays the most efficient cell and it achieves a PCE of 25.6% (Table 2).

Table 2. Record efficiencies for silicon solar cells.Source: Martin A. Green et al., 2014, "Solar cell efficiency tables (Version 45)".

Classification	Efficiency (%)	Area (cm ²)	V _{oc} (V)	J _{sc} (mA/cm²)	Fill factor (%)	Test centre (date)	Description
Silicon							
Si (crystalline)	25.6±0.5	143.7 (da)	0.740	41.8	82.7	AIST (2/14)	Panasonic HIT, rear junction
Si (multicrystalline)	20.8±0.6	243.9 (ap)	0.6626	39.03	80.3	FhG-ISE (11/14)	Trina Solar
Si (thin transfer submodule)	21.2±0.4	239.7 (ap)	0.687	38.50	80.3	NREL (4/14)	Solexel (35 µm thick)
Si (thin film minimodule)	10.5±0.3	94.0 (ap)	0.492	29.7	72.1	FhG-ISE (8/07)	CSG Solar (<2 µm on glass; 20 cells)



In spite of the improvements in silicon solar cells efficiences over many years, scientists affirm to be very close to the limit of silicon's capability. As it was explained, the record efficiency of 25% for silicon cells was unbroken from 1999 to 2014, which shows the slow evolution in the last years.

Other known PV technologies not based in silicon are or low-efficient or enormously expensive. If solar wants to become the future of global energy supply, the need of research for other alternative technologies is unquestionable.



2.2 Perovskite solar cells

2.2.1 The new promising technology for solar PV

Among all the latest research in the field of photovoltaics, experts refer to perovskite solar cells as the revolutionary technology for solar. Perovskite is the number one in the list of alternatives to substitute the stagnant silicon as semiconductor material in solar cells.

Other relatively recent researches are based on organic compounds, instead of inorganic materials like silicon. Organic materials are very cheap to manufacture, which is very important to compete in the energy market. On the other hand, researchers do not achieve high efficiencies with these materials and their long-term stability is really low.

The ideal would be to combine the low cost of organic compounds with the high performance and lifetime of inorganic materials. Here is where perovskite becomes promising, as it already combines two of these desired qualities. Hybrid organic-inorganic perovskite solar cells developed to date are low cost and high-efficient but the long-term stability problem still needs to be solved.



Figure 8. Perovskite solar cell efficiencies vs. other technologies. Source: Ossila, 2014, "Perovskites and Perovskite Solar Cells".

The main reason why perovskite technology is now such a big excitement in photovoltaics is how fast it has developed. Researches about perovskite application for PV started in 2009 when Kojima et al. created a perovskite cell with a first PCE of 3.8%. By November 2014, a certified PCE of 20.1% was already achieved by KRICT (Korean Research Institute of Chemical Technology). Experts estimate continuous improvements that will keep increasing the power conversion efficiency of perovskite solar cells over the coming years.



2.2.2 The material: Perovskite

First of all, it is necessary to clarify that in this paper perovskite is referred as a structure more than a material itself. In theory perovskite is a mineral composed of calcium titanate (CaTiO3), which was discovered in the Ural Mountains in 1839, but the word perovskite is also used for any other material compound with the same type of crystal structure as the perovskite mineral.

This generic perovskite structure has the chemical formula ABX3, where A and B are cations (ion with positive charge) and X is an anion (ion with negative charge). One large B cation is in the center of the cubic structure surrounded by six X anions in the faces of the cube forming an octahedron, and finally one A cation is located in each of the eight corners of the cube.

Depending on the atoms or molecules that are used in this structure, perovskites can have a lot of different interesting properties.



Figure 9. Crystal structure of perovskites. Source: Samuel D. Stranks et al., 2015, "Formation of Thin Films of Organic-Inorganic Perovskites for High-Efficiency Solar Cells".

The predominant perovskite solar cell to date uses CH₃NH₃PbI₃ as semiconductor. The cations CH₃NH₃ is methylammonium, Pb is a cation of lead and the anions I₃ are triiodide. First researchers in perovskite solar cells also tried to use tin (Sn) instead of lead, but lead resulted to be much more efficient. Another possible halides for the anions are chlorine (Cl) and bromine (Br), but again iodide (I) was the most interesting option.

As the perovskite used in this new type of solar cell is not the mineral but the structure and the required metal to produce it is lead, then lead is the material of interest. Lead is most commonly extracted from mineral rocks called ores which also contain copper, zinc or silver. Galena (PbS) is the main lead mineral, followed by anglesite (PbSO4) and cerussite (PbCO3).

Other common materials in the architecture of a perovskite solar cell are, like in silicon cells, titanium dioxide (TiO2) for the anti-reflection coating, an aluminum frame and a glass cover. In the same way, metals such as silver-palladium (Ag-Pd), nickel (Ni) or copper (Cu) are also needed for the electrical contacts.



There are two main different structures for the organic-inorganic perovskite solar cells (Figure 10). First, there is the simple planar heterojunction where the perovskite layer is placed between the n-type and p-type contacts. Secondly, there is the mesostructured cell where the perovskite layer is infiltrating a mesoporous metal oxide usually made of titanium dioxide. Both of these architectures are being nowadays developed but they will probably converge in one single structure during the next years.



Figure 10. Schematics of the planar and mesostructured device architectures. Source: Samuel D. Stranks et al., 2015, "Formation of Thin Films of Organic-Inorganic Perovskites for High-Efficiency Solar Cells".

Some of the qualities that make perovskite solar cells so interesting are, firstly, that they are cheap to produce, and secondly, that these cells have very beneficial optical and electronic properties. Besides, perovskite has high flexibility and it is a good light absorber over the whole visible solar emission spectrum.

Materials in perovskite cells have effective diffusion lengths over 100nm for both electrons and holes, which is relatively large and means that they can work properly in a thin-film structure. Additionally and not less important, perovskites display high charge carrier mobility and high charge carrier lifetime, which is important for light-generated electrons and holes moving far enough to be extracted as current without losing their energy in form of heat inside the solar cell.



2.2.3 Formation of perovskite solar cells

The simple and cheap methods to manufacture perovskite solar cells are undoubtedly one of the best advantages over the silicon cells. Low cost is possible because fabrication techniques need low temperatures and so a low energy consumption. Typical silicon cells processing require temperatures over 1000°C and special room facilities to purify silicon, making it much more expensive.

Two methods are used to prepare the perovskite layers for perovskite solar cells:

- Solution processing, which is itself divided in two similar but different techniques.
- Vacuum evaporation process.

These perovskite deposition techniques form the perovskite material by the component combination of organic methylammonium iodide (CH₃NH₃I) with the inorganic lead(II) iodide (PbI₂).

In the two processes using a solvent, perovskite is deposit on a substrate by spin-coating. One of the processes makes this spin-coating in one step and the other solution process in two steps. Schematics of these procedures are shown in Figure 11.



Figure 11. Coating procedures to deposit perovskite films. Source: Hyun Suk Jung and Nam-Gyu Park, 2014, "Perovskite Solar Cells: From Materials to Devices".

One-step coating technique dissolve CH₃NH₃I and PbI₂ in a proper solvent and then this solution is coated onto the substrate. On the other hand, in the two-step coating technique the PbI₂ is first dissolve and coated on the substrate, and then, another solution of CH₃NH₃I is coated on the PbI₂ film. In Figure 11, DMA, DMF and IPA are the solvents and they represent dimethyl acetamide, dimethyl formamide and isopropyl alcohol, respectively.



It was found that perovskites made by two-step coating have a better morphology and interfaces that those made by the one-step method, so that they display a higher photovoltaic performance.

Regarding to the vacuum evaporation process, CH₃NH₃I and PbI₂ are co-evaporated at around 150°C to prepare the perovskite film. This method is more expensive than solution processing but it has some advantages. The thickness control and uniformity of the film is much better than with solution-processed layers. Moreover, vacuum evaporation technique uses less solvents so that it reduces the risk of solvent remnants.



Figure 12. Perovskite film fabricated on a glass sheet. Source: Boshu Zhang, Wong Choon Lim Glenn & Mingzhen Liu, 2013.

Commercialization of perovskite solar cells is still challenging but some start-up companies are already promising the first perovskite modules on the market by 2017.

It should be pointed out that another attractive possibility for perovskite films is to include them in tandem solar cells based on traditional silicon devices. In these two-level tandem configurations, perovskites would be as top cells while crystalline silicon would be as bottom cells. According to Michael Grätzel in his article *"The light and shade of perovskite solar cells"* (2014), power conversion efficiencies of 28% to 30% appear to be easily attainable with these tandem cells.



3. THE PROBLEM

The fossil fuels dominance is coming to its end in a not so long term, because their earth reserves are finite. It is becoming urgent to find alternative energy sources and solar is one of the most attractive candidate to be this alternative since it is renewable, unlimited and with enough potential to supply all the world energy demand. Therefore, major future investments are needed to develop the photovoltaic technology. However, current silicon-based technologies have certain limitations that hinder the PV development. New materials such as the now famous perovskite are being investigated to overcome these limits. Some viability aspects for the material uses are analyzed in this study.



Figure 13. Estimation for global cumulative PV capacity (2014-2018). Source: EPIA, 2014, "Global Market Outlook for Photovoltaics 2014-2018".

As it is already explained in 2.1.1., silicon metal is relatively easy to obtain as the supply of the minerals from which it is made is practically inexhaustible and its process is not very expensive. What is expensive is the process to produce the final grade silicon required for solar cells manufacturing. Furthermore, grade silicon production is limited to the number of purifying installations where this process can be carried out. That is one of the limits to the growth of silicon use in photovoltaics.

In consequence, future investments in photovoltaic should consider if it is worthy to invest on new purifying installations to increase the supply of monocrystalline and polycrystalline silicon or if it is more interesting to invest in the development of perovskite solar cells. The investments share for silicon and perovskite technologies is analyzed for different scenarios in the results.

Another and not less important barrier to expand the use of silicon in PV cells is about the limit of power conversion efficiency (PCE) in silicon solar cells. There are clear evidences of a



bigger potential to rise the PCE in solar cells using perovskite. Moreover, it is more important to increase the efficiencies than reducing more and more the costs of materials because even if these costs become really small, other considerable costs like installations and maintenance will remain. Low costs are important, but high efficiencies are more, and perovskite cells seem to combine both qualities.

Therefore, for the probable case where the investments are targeted mainly to commercialize and improve perovskite solar cells, this study also analyzes if raw material resources are enough to supply a future large-scale production. Lead is the main element involved in the perovskite structure of these promising cells, so it is the material to focus the analysis, together with silicon.

There are some concerns about the use of lead in solar cells because of its environmental impact. The quantities of lead needed to satisfy the future production of perovskite solar cells are estimated in different scenarios. This lead consumption for photovoltaics is compared with the global lead consumption in order to check whether it is significant or not.

Another issue that is considered in this paper is how evolves the amount of recycled material compared to the new extracted, both for silicon and lead. So it is analyzed, in economic terms, the appropriate fraction that should be recycled for each material during the next decades.



Figure 14. Recycle solar panels. Source: SUNPRO Energies.

Summing up, the problems and issues that are analyzed and commented in the results obtained in this study are:

- Verification of the global growth of photovoltaics in the future.
- Investment share for silicon and perovskite technologies. It is checked if it is worthy to invest in perovskite solar cells rather than in traditional silicon cells.
- Possible scarcity of the material resources.
- Amount of materials to be recycled and so the recycling fraction for each material.
- Significance of the lead environmental impact due to perovskite solar cells production.



4. THE METHOD: SYSTEM DYNAMICS

The chosen method to carry out the analysis in this paper is System Dynamics. According to John D. Sterman, this methodology can be applied to any dynamic system with any time and spatial scale.

The method itself consist in building a simulation model with stocks and flows that reproduces the reference mode of a system based on historical data. Then, once the model is validated, it is used to simulate the behavior of the system over time.

The principal aim of this technique is to understand the structure and the behavior of a complex system in order to be able to analyze its problems and how it would be affected in the future under different conditions.

Nevertheless, it is important to point out that it is extremely hard to create a model that replicates exactly the behavior of a system. A lot of approximations are made in the parameters values and in the structure during the building of a dynamic model. Testing is necessary to make these approximations the most accurate possible. The quality of data collection is also a very important factor to create a useful model.

Systems Dynamics is an appropriate method for this study because the use of materials in photovoltaics is a non-linear system that is influenced by a big amount of elements with a lot of relationships between them, creating then reinforcing and balancing loops. These feedback loops and their entailed time delays are clearly reproduced through this modelling technique. Moreover, all the software products available to create this type of models allow to easily modify the parameters of the system to run simulations in different scenarios and test several situations.

The software used to build the system dynamic model for this analysis is *iThink 10.0.6*, developed by the company *isee systems*.



5. HYPOTHESIS

The hypothesis for this study is that, because of an awaited major growth of solar energy in the world, the need of materials to produce solar panels will strongly increase so that their consumptions may become significant and there could be problems of scarcity in the future. It is not supposed to find a scarcity problem for silicon since it is immensely abundant but it would be probably found a problem with resources of lead due to the growth of perovskite solar cells. Then, it would be expected a big rise in the recycling fraction of lead and a reduction of its extraction rates to face this scarcity problem.

In fact, it is also expected an important investment in the perovskite technology so that it would perform a huge development to rapidly become dominant over the traditional silicon technology.

Another hypothesis for the expected results is that the environmental impact from the lead used in perovskite solar cells production would be negligible if it is compared to other lead consumptions in the world.

5.1 Previous premises

As a result of the hypothesis, the first premise made before building the system dynamic model used for the analysis is that investments in photovoltaics will progressively increase in order that solar becomes the main global source of energy in a long term. These energy policies will be adopted by most of governments in the future. Otherwise, if finally solar does not succeed, all the issues discussed in this paper have no need to be analyzed.

The next important assumption made in advance is that all the existing challenges for the successful commercialization of perovskite solar cells will be solved in the coming years, especially the concerns about their lifespan and environmental impact. Here there are some arguments to carry out this optimistic assumption:

Long-term stability of perovskite solar cells cannot be still guaranteed because the
organic compound of the perovskite material is soluble in water and it provokes that
the cell deteriorates rapidly in contact with water, for example when it rains. Some
encapsulating techniques are already being investigated to prevent this fast degradation
of the material in moist environments.

Furthermore, this problem has to be certainly resolved since nobody would be interested in buying perovskite solar cells just with a short-term stability because people do not want to change the cells frequently. Perovskite solar cells should have more than 20 years of operation lifetime to be able to be commercialized. A lifetime of 22 years is estimated for perovskite cells in the model, a bit less than the 25 years lifetime average for silicon cells. Anyway, the value of perovskite cells lifetime can be varied in the model through a slider to simulate different scenarios.





Figure 15. Water drops over a solar panel. Source: Hawaii Renovation, 2014, "Green-friendly sealing and cleaning".

About the environmental impact of lead, this metal is toxic for living beings and it can enter and move through ecosystems by different sources. As first assumption this issue is simply ignored because it is used in very small quantities compared to other industries like batteries. However, as it is said in chapter 3, it is one of the problems that are treated here. The lead consumption to produce perovskite solar cells that is obtained in the results of the model is compared with the world total lead consumption, so that it is possible to confirm if it is appropriate to ignore its impact or not.

Moreover, according to Jack Lifton in his article "*Materials for Solar Photovoltaics Cells I: Silicon, Very Abundant, Very Expensive*" (2008), it takes a lot of chemical processing to produce pure silicon from which to ultimately make a PV solar cell, and that uses and produces an enormous amount of carbon dioxide, carbon monoxide, chlorine and so forth. It can then be said that use of pure silicon has also a considerable environmental impact.

Finally, the last previous premise made is that power conversion efficiency (PCE) of perovskite solar cells will keep increasing fast and it will achieve the high-efficiencies expected in the coming years. A very good cost-effectiveness ratio for perovskite cells is undoubtedly assumed. In the model, it is estimated a future PCE average of 40% for commercialized perovskite solar cells. Anyway, as for their lifetime, the value of this PCE can be varied in the model through a slider to simulate scenarios with different reached efficiencies.



5.2 Assumptions and limitations for the model

In the first place, as it is already said in sections 2.1.1. and 2.2.2., the analysis is focused on the main material of each technology. As the two technologies here studied are silicon solar cells and perovskite solar cells, silicon and lead (for perovskite) are the only materials considered in the model. It is assumed that the other materials required to produce solar cells are needed in really low quantities or they are considerably abundant.

Note that, in case of need to analyze other materials, the model could be easily adapted and used for a different material than silicon or lead.

It is also important to point out that when it is talked about silicon solar cells in this model, it is meant to be the most common silicon cells in the market. As it is said in the section 2.1.2., these are the polycrystalline silicon cells (multi-Si).

The global investments in solar energy obviously depend on the world GDP since part of it is destined to these investments. The model uses a constant percentage of world GDP that is invested in solar energy (0.150411%), which is the real percentage of the year 2013 according to data extracted from REN21 in its "*Renewables 2014 Global Status Report*" (2014). Actually, this percentage should vary during the years but it will remain constant in the model.

Consumption of silicon and lead in other sectors may also vary in the future but the model use constant values for these other consumptions, which are the annual average consumptions of each material in the last years.

Some other assumptions made as a result of the lack of data are:

• Extraction, processing and recycling costs of materials change according to the amounts of accumulated production and accumulated recycling. There is an important lack of data for this type of costs, but this is not a big problem since their exact monetary values are not the point to deal with. These costs are only used in the model to be compared between them.

In consequence, a scale from 0 to 10 has been defined for all these costs and they are, therefore, unitless. Units are not relevant because the costs are always compared in form of fractions so that their units are canceled.

The variation of the recycling fraction of each material only depends on the extraction cost compared to the cost of recycling. So the fraction of recycling just changes due to economic aspects. Other factors, like social and environmental, are not taken into account because it would be really difficult to define correctly this kind of parameters since recycling methods and policies may differ a lot between countries.



- Material needs are calculated in volumetric units and then transformed to units of weight using the pure material density. It is done this way because it is not found data about the quantities in weight of materials required to produce a defined solar cell.
- The obtained amounts of needed material are adjusted by waste rates. Silicon waste rates have been taken from the paper "Silicon processing: from quartz to crystalline silicon solar cells" (2011) by B.S. Xakalashe and M. Tangstad. However, data for lead waste rates in perovskite solar cells cannot be found. Lead waste rates may not be exactly equal to silicon waste rates but in the model they are supposed to be the same.

All these considerations and assumptions manifest the existing limitations of the model and the analysis.



6. THE MODEL: STOCK AND FLOW DIAGRAM

The stock and flow diagram built for the analysis replicates the evolution of solar energy from 2004 to 2013 at a global level and then it simulates until the year 2050 (Figure 16). The model simulation starts in 2004 because before photovoltaic energy had a really small market and there is not a lot of data from the previous years.

🕖 Run Spec	S		X				
Length of sin	Length of simulation:						
From:	2004	Hours					
		Days					
To:	2050	Weeks	Interaction Mode:				
DT.		Months	Normal				
DT:	0.25	Quarters	Flight Sim				
Pause	DI as fraction	Years					
interval:	INF	Other					
Integration M	lethod:	Sim Speed:					
Euler's	 Euler's Method Runge-Kutta 2 		ecs = 1 unit time				
Rung			4.6 secs				
Rung	e-Kutta 4						
🔽 Analyze 🛚	Analyze Mode: stores run results in memory (0.1 MB required)						
			Cancel OK				

As said in the section 4, the software used to create the system dynamic model is *iThink 10.0.6*.

Figure 16. Run Specs for the simulation.

The model is focused in the consumption of silicon and lead needed to produce all the solar cells required for the capacity demand determined by the investments of governments.

Some parameters or equations differ for the two technologies analyzed in the model so one array dimension "Technology" is created with two element labels: "WithSilicon" and "WithPerovskite" (Figure 17).

Array Editor						X
Array dimensions:	ions:			Dimension element labels:		
Name	Indexed by	Size	*	WithSilicon	*	
Technology	Label	2		WithPerovskite		

Figure 17. Array dimension for the two technologies analyzed in the model.



For a better understanding of the model building, the Figure 18 shows a very basic Causal Loop Diagram (CLD) of the system. The main loops in the model are the two reinforcing loops R1 and R2.

Note that every element with the word "MATERIALS" represents two elements in the model: one for silicon and one for lead. Similarly, the elements which are "per Technology" are arrays with the two dimensions defined previously in Figure 17. So this basic CLD is a two dimensions diagram. Some relations depend actually on the comparison between the same elements of each material. For example, when costs of extracting or recycling silicon increase compared to the costs of lead, the investments for the silicon technology will decrease but the investments for the technology using perovskite lead will increase.



Figure 18. Basic Causal Loop Diagram of the system.

The meaning of the black arrow from "Produced MATERIALS" to "Cost of extracting and processing MATERIALS" is that its polarity may change. At the beginning this cost decreases when the accumulated production increases but, when this production becomes too high and problems of scarcity appear, the extraction cost may rise.

More detailed Casual Loop Diagrams are shown in the section 6.3.



6.1 Building the model

In this section it is explained step by step how the model is built and the relationships between all the stocks, flows and converters.

First of all, there are the stocks of material in use for each technology, together with their inflows and outflows (Figure 19). The initial values for these stocks are 0 since the production of solar cells in 2004 is negligible compared to the current one or the estimated one for the future. Units for the stocks are million tons (MT) and so MT/year for the flows.



Figure 19. Material in use.

The outflows of used material represent the silicon and perovskite lead from the consumed cells, so the time to become used is the respective lifetime of these solar cells (in years). The general equation for these outflows is:

$$Material used [MT/year] = \frac{Material in use [MT]}{Lifetime cells [years]}$$

Lifetime for perovskite solar cells can be modified with a slider, as it is already explained in the section 5.1.

As shown in Figure 20, the inflows of new material for solar cells production are given by the material needs, which are calculated in units of volume (m³/year). The units of needed material are converted to weight multiplying by the material density and then a unit converter is used to change from kilograms to million tons.

New material for solar
$$\left[\frac{MT}{year}\right] = \frac{Material needs \left[\frac{m^3}{year}\right] * Material density \left[\frac{kg}{m^3}\right]}{Unit converter \left[\frac{kg}{MT}\right]}$$



The obtaining of silicon needs and perovskite lead needs is explained later in this section.



Figure 20. New material for solar cells production.

Some fraction of the material used in old solar cells, together with the material consumed annually in other sectors, is recycled (Figure 21). Recycling is very important in order to make solar energy sustainable, since material resources are not unlimited like sunlight.



Figure 21. Recycling rates of material.



Recycling rates for each material (in MT/year) are determined by the sum of total material consumption multiplied by their respective recycling fraction.

```
Recycling rate = (Material used + Other consumption) * Recycling fraction
```

The stocks of recycled material accumulate all the material that is recycled during the simulation. Their initial value is 0 and their units are million tons.

These recycling rates are also used to define the extraction rates of each material (Figure 22).



Figure 22. Extraction rates of material and accumulated production.



The equation for the extraction rates (in MT/year) is:

Extraction rate = New material for solar + Other consumption – Recycling rate

All the material that is extracted and produced throughout the simulation is accumulated in the stocks of produced material. As for the stock of recycled material, their initial value are 0 and their units are million tons.

From these stocks is determined the evolution of the extracting, processing and recycling costs (Figure 23 and Figure 24, respectively) for each material. In this case, relations between these variables are defined by graphical functions instead of equations.



Figure 23. Cost of extracting and processing material.

New material extraction involves a high processing to obtain the form of material required for the solar cells production, especially in the silicon technology where metal silicon needs several expensive treatments to become pure grade silicon. The high cost of this processing is quite passed on to the ultimate solar cells price.



Figure 24. Cost of recycling material.

As it is explained in the assumptions made in the section 5.2, these costs are unitless and their values are in a scale from 0 to 10.

The shape of each graphical cost function due to the growth of accumulated production and recycling has been established after a lot of testing. At the beginning, the cost of extraction decreases with more accumulated extracted material because of learning and technical improvements, but at some point it starts to increase due to scarcity. The behavior in the graphical function of recycling cost is that it decreases when accumulated recycled material grows because the recycling techniques ameliorate.

The next figures (Figure 25 to Figure 28) display the graphical functions for all these costs of extracting-processing and recycling.




Figure 25. Graphical function for cost of extracting and processing silicon.

The cost of extracting and processing silicon for solar cells does not vary so much because its technology has already been very developed since 2004. However, for lead used in perovskite solar cells the cost is strongly reduced with experience and it reaches the expected low cost for the material, which becomes more than half of silicon cost.



Figure 26. Graphical function for cost of extracting and processing lead.





Figure 27. Graphical function for cost of recycling silicon.

Recycling functions are very similar for silicon and lead. Nonetheless, cost of recycling lead is considered slightly smaller than for silicon since the general technology required to produce perovskite solar cells is supposed to be cheaper.



Figure 28. Graphical function for cost of recycling lead.



Then, the fraction recycling for silicon and for lead depend on their respective costs of extracting-processing and recycling (Figure 29).



Figure 29. Fraction recycling for silicon and lead.

Recycling fractions are also coming from graphical functions and they vary according to the relative cost of recycling compared to the cost of extracting.

$$Fraction \ recycling = \ f\left(\frac{Cost \ of \ extracting \ and \ processing}{Cost \ of \ recycling}\right)$$

These graphical functions are shown in the next figures (Figure 30 and Figure 31). The fraction of recycling is kind of stabilized when the costs of extracting-processing and recycling are close, but it increasingly decreases when the recycling cost is relatively high and vice versa. If the cost of extracting and processing is more than double of the cost of recycling, all the used material will be recycled and so the recycling fraction will be equal to 1.



Figure 30. Graphical function for fraction recycling silicon.



Both graphical functions have almost the same shape, similar to the curve of the *logit function*, but the average recycling fraction of silicon is higher because it has been used a longer time in solar cells production so that it is more commonly recycled nowadays.



Figure 31. Graphical function for fraction recycling lead.

Furthermore, there is another sector in the model to decide the total annual investments in solar energy (Figure 32). This investments are determined by multiplying the world GDP by the percentage of world GDP invested in solar energy and a fraction of the cost of fossil fuels compared to the adjusted cost of solar energy. Units used are billion US Dollars.



Figure 32. Total investments in solar energy.



There is also a slider "Scenario effect on investments" with a scale from 0.5 to 1.5 and an initial value of 1. This effect on investments is used to simulate the model in different scenarios where the investment policy can be more or less strong.

The global "Adjusted Cost of solar energy" (Figure 33), in US Dollar per megawatt-hour (US\$/MWh), is calculated by the multiplication of the estimated basic cost of solar energy and a technological adjustment that is proportional to the investment share for each technology.



Figure 33. Adjusted cost of solar energy.

This unitless "Adjustment in cost of solar energy" (Figure 34) is equal to the fractional comparison between the costs of perovskite technology and the costs of silicon technology. The compared costs for each technology are calculated by this equation:

Costs Tech. = [Cost of extracting and processing * (1 - Fraction recycling) + Cost of recycling * Fraction recycling]

Then, the final adjustment is:



Figure 34. Adjustment in cost of solar energy.



It should be pointed out that this adjustment is only applicable to the proportional cost of solar coming from the perovskite technology, since for the silicon one the cost does not need to be adjusted as it is commensurate to the basic cost of solar energy. The value of the adjustment is always equal to 1 for the proportional cost of solar coming from the silicon technology.

So the adjustment brings down the global cost of solar energy if perovskite technology is cheaper than the traditional silicon one and if there is a higher investment share put in perovskite cells.

In regard to the "Investment Share per Technology" (Figure 35), this variable is determined through a *logistic function*. This *logistic function* is defined by a parameter alpha (α) and depends on the difference between the costs of extracting and processing in each technology. Investment share represents a fraction from 0 to 1 and it does not have units.



Figure 35. Investment share per technology.

The general equation for this indicated investment share on the technology "i" (ISi) is:

$$IS_i = \frac{e^{-\alpha \cdot C_i}}{\sum_{j=1}^N e^{-\alpha \cdot C_j}}$$

Where C_i or C_j are the cost of extracting and processing the material for the technology "*i*" or "*j*" and *N* is the total number of different materials.

Moreover, it must be satisfied that the sum of the investment shares is equal to 1 (or 100%):

$$\sum_{i=1}^{N} IS_i = 1$$
 (100%)

So in this case N=2 and, for the indicated investment share on the perovskite technology, in this equation "i" represents the lead for perovskite and "j" represents silicon. Then, the investment share on the silicon technology is the simply difference from the investment share on perovskite technology to the 100%.



Figure 36. Logistic function for IS(perovskite) for C(silicon)=6 with different alpha (α).

For a cost of extracting-processing silicon equal to 6 in its 0-10 scale, the *logistic function* for the investment share on perovskite technology is represented in Figure 36 for two different parameter alpha (α).

In the model, the parameter alpha (α) is a slider from 0 to 1 with an initial value of 0.5. The higher is this parameter, the higher is the sensitivity in the variation of the investment share. The model uses an alpha (α) of 0.5 because a stronger sensitivity would make the investment share on perovskite to tend to 1 excessively fast.

From the investment share and the total investments in solar is determined the variable "Investments per Technology" (Figure 37) in billion US Dollars, which is the amount invested in each photovoltaic technology.



Figure 37. Investments and Capacity per Technology.



The obvious formula for these investments is:

Investments per Tech. = Total Investments in solar * Investment Share per Tech.

Figure 37 also shows that from these investments and an adjustment with the solar cells efficiency of each technology, it is set the new "Capacity per Technology" through a graphical function (Figure 38). Units for this new PV capacity are gigawatts per year.

Capacity per Tech. = f(Investments per Tech. * (1 + Efficiency of solar cells))



Figure 38. Graphical function for Capacity per Technology.

The converter "Efficiency of solar cells" (Figure 39) is just an array which contains in its two dimensions the power conversion efficiency (PCE) of the solar cells in each technology.



Figure 39. Efficiency of solar cells.

Note that, as it is already said in the section 5.1, the estimated efficiency of perovskite solar cells is a slider that can be varied to simulate different scenarios.



The efficiency of the different solar cells, together with the received sunlight energy, gives the "Converted electrical energy" (Figure 40). The received sunlight energy used here is the daily average of incident solar energy over the entire earth, in watts per square meter (in watts/m²), and it can be varied with a slider.



Figure 40. Converted electrical energy.

This converted energy is the electricity in watts that is produced in average from each square meter (m²) of each type of solar cell, so its units are watts/m². This variable is then used in the model to fix the material needs for each technology.



Figure 41. Material Needs: silicon and perovskite lead.



Indeed, the important variables "Silicon Needs" and "Perovskite Lead Needs" (Figure 41) are first determined by the division of the new capacity per technology by the converted electrical energy, so that it is given the surface of solar cells (in square meters, m²) required to build all the new demanded capacity. After that, this is multiplied by the thickness of the material layer in order to obtain the volume of needed material in cubic meters (m³). This volume is then adjusted by the waste rates of material during its production process. In the next section 6.2 it is explained the calculation of this waste adjustment.

In addition, the capacity is previously converted from gigawatts/year to watts/year through a unit converter so that it has the same energy units that the converted electricity. The units of the material needs are cubic meters per year (m³/year), afterwards converted to tons per year as it is previously shown in the Figure 20.



Figure 42. World Total Solar Capacity.

Finally, there is a sector with the world total solar capacity (Figure 42) where the "Total Solar Capacity" (in gigawatts) is a stock whose inflow is the new built capacity and whose outflow it the lost capacity per year by scrapped cells.

The new capacity is just the addition of the new annual capacity for each technology and the scrapped capacity depends on the average lifetime of solar cells, which is proportional to the existing cells by technology.

The full simulation model is shown in the Appendix A of this paper together with its equations in the Appendix B.



6.2 Data collection

In this section it is described all the data used in the model. First it is important to point out that, in the whole model, the monetary unit is US Dollars (US\$) and it is not adjusted by inflation. On one hand, there are some elements that vary over the years. On the other hand, most elements are constant or they are considered to keep constant.

6.2.1 Variables

To begin with, a main variable is the world GDP which is used to calculate the total investments in solar energy. Table 3 shows the data for the world GDP (in billion US\$) collected from the free data of *Knoema*, who used as source the "World Development Indicators" (April 2015) generated by *The World Bank*.

World GDP	
Year	Billion US\$
2004	43 412
2005	46 965
2006	50 880
2007	57 328
2008	62 858
2009	59 539
2010	65 217
2011	72 140
2012	73 514
2013	75 593

Table 3. World GDP in constant 2005 US\$ (2004-2013).Data source: The World Bank, 2015, "World Development Indicators (WDI)".

Table 4. Cost of fossil fuels (2004-2013).

Data source: US\$/GJ are graphically determined. Then, converted from GJ to MWh.

Cost of fossil fuels		
Year	US\$/GJ	US\$/MWh
2004	45.00	161.87
2005	48.00	172.66
2006	51.00	183.45
2007	55.00	197.84
2008	53.00	190.65
2009	52.00	187.05
2010	50.00	179.86
2011	51.00	183.45
2012	50.00	179.86
2013	49.00	176.26



Table 5. Cost of solar energy (2004-2013).Data source: US\$/GJ are graphically determined. Then, converted from GJ to MWh.

Cost of solar energy		
Year	US\$/GJ	US\$/MWh
2004	160.00	575.54
2005	150.00	539.57
2006	155.00	557.55
2007	140.00	503.60
2008	125.00	449.64
2009	105.00	377.70
2010	90.00	323.74
2011	80.00	287.77
2012	70.00	251.80
2013	60.00	215.83

The costs of fossil fuels and solar energy in US\$/GJ (Table 4 and Table 5, respectively) are approximately determined from the graph shown in Figure 43 and contrasted with other graphs and tables. After that, gigajoules (GJ) are converted to megawatts-hour (MWh) because the units used for these costs in the model are US\$/MWh. The conversion is 1 GJ = 0.278 MWh.

The name of these energy costs is "Levelized Cost Of Electricity" (LCOE), which is the net present monetary value of electricity over the lifetime of the energy production.



 $LCOE = \frac{Total \ Life \ Cycle \ Cost}{Total \ Lifetime \ Energy \ Production}$

Figure 43. Historical comparison of the price of solar energy with the price of the conventional energy sources (in US\$/GJ). Source: Brian McConnell, 2013, "Solar Energy: This is What a Disruptive Technology Looks Like".



This inaccurate graphical approximation is the way used to determine the levelized costs of energy because it is very difficult to find exact data for these unit costs at a global level, especially for solar energy. Another difficulty is the fact of looking for a general cost of fossil fuels when cost varies between the different types of this nonrenewable energy source, so it is needed to make an approximate average for these different types.

Efficiency of silicon solar cells	
Year	PCE (%)
2004	15.0%
2005	15.5%
2006	16.1%
2007	16.7%
2008	17.4%
2009	18.2%
2010	19.0%
2011	19.9%
2012	20.9%
2013	22.0%

Table 6. Efficiency of silicon solar cells (2004-2013).Data source: approximate weighted average for all the commercial silicon solar cells.

The last variable element is the power conversion efficiency of silicon solar cells (Table 6). It is important to note that this PCE is an approximate average of all the commercialized silicon solar cells, proportionally to the market share of each type of silicon cell.



6.2.2 Constants

Regarding to the constant elements in the model, the Table 7 collects all of these data values together with their sources. Some of these constants are directly taken from a specific source while other constants are approximations or they are simply based on premises held from the expectations.

The "Scenario effect on investments" is just a slider created to simulate different investment policies in the system and the "Parameter alpha for logistic function" is an element needed to define the investment share per technology which is fixed after testing and according to the required sensitivity of the *logistic function*.

DATA COLLECTION FOR CONSTANTS			
Data Name	Value	Unit	Source
Lifetime silicon cells	25	Years	Energy Informative, 2014, "The Real Lifespan of Solar Panels"
Lifetime perovskite cells	22 *	Years	-
PCE perovskite cells	40 *	%	-
Silicon layer thickness	0.0001	Meters	C. Honsberg and S. Bowden, "Silicon Solar Cell Parameters"
Perovskite layer thickness	0.0000005	Meters	Gary Hodes, 2013, "Perovskite-Based Solar Cells"
Silicon density	2 329	Kg/m³	Wikipedia, "Silicon"
Lead density	11 340	Kg/m³	Wikipedia, "Lead"
Waste material adjustment	0.168	Unitless	B.S. Xakalashe and M. Tangstad, 2011, "Silicon processing: from quartz to crystalline silicon solar cells"
Received sunlight energy	164 *	W/m²	Professor Gregory Bothun (University of Oregon)
Other silicon consumption	1.55	MT/year	Minor Metals Tarde Association (MMTA), "Silicon Market Overview"
Other lead consumption	8	MT/year	Wikipedia, "Lead"
Pctg of world GDP invested in solar energy	0.150411	%	REN21, 2014, "Renewables 2014 Global Status Report".
Scenario effect on investments	1 *	Unitless	-
Parameter alpha for logistic function	0.5 *	Unitless	-

Table 7. Data collection for constants.

*Note: the values of these constants are sliders in the model, so that they can be easily varied to simulate the system behavior in different scenarios. The values in this table represent their initial value in the model.



On one hand, the lifetime of silicon solar cells is defined according to this affirmation made by the guide Energy Informative in its paper "*The Real Lifespan of Solar Panels*" (2014):

"The majority of manufacturers offer the 25-year standard solar panel warranty, which means that power output should not be less than 80% of rated power after 25 years."

On the other hand, both lifetime and efficiency of perovskite solar cells are simply based on premises held from the expected values to be reached. Anyway, these two constants can be varied through a slider for the model simulation.

About the layers thicknesses, C. Honsberg and S. Bowden state in the section "Silicon Solar Cell Parameters" of PV Education that "an optimum silicon solar cell with light trapping and very good surface passivation is about 100 μ m thick". For perovskite layers, Gary Hodes says in his article "Perovskite-Based Solar Cells" (2013) that the perovskite film thickness is about 500 to 600nm.

Furthermore, the densities for silicon and lead are taken from the articles "*Silicon*" and "*Lead*" in Wikipedia. These densities are the ones defined near to a room temperature, which is approximately 20°C.

The value for the "Waste material adjustment" is calculated using three waste rates in the production process of silicon solar cells, which are taken from the article "*Silicon processing: from quartz to crystalline silicon solar cells*" (2011) by B.S. Xakalashe and M. Tangstad. The values of these three waste rates are:

- 70% wasted from quartz to metallurgical-grade silicon.
- 20% wasted from cutting the silicon ingots.
- 30% wasted from wafering, as saw dust kerf loss.

Then, the final value for the waste material adjustment is:

Waste material adjustment =
$$(1 - 0.7) * (1 - 0.2) * (1 - 0.3) = 0.168$$

The same waste rates are assumed for lead in the production of perovskite solar cells.

The constant "Received sunlight energy" is, as it is already defined in the section 6.1 and according to the professor Gregory Bothun from the University of Oregon, the daily average of incident solar energy over the entire earth (in watts/m²).

Even if the sunlight energy arriving to the earth's surface when the sun is at the zenith is about 1050 watts/ m^2 , it is necessary to consider other factors like the hours of light in a day, the clouds and other climatological conditions. After all these considerations, professor Gregory Bothun obtained a sunlight energy of 164 watts/ m^2 received on the Earth's surface.



According to the Minor Metals Tarde Association (MMTA) in its report "*Silicon Market Overview*", in 2010 the consumption of silicon is about 1.76MT/year and around 12% of it is used in photovoltaics. So it is easy to calculate that the consumption in other sectors is 1.55 million tons per year.

The annual average consumption of lead is about 8MT/year. As perovskite cells are really recent, it is assumed that all the 8 million tons per year are consumed in other sectors.

Note that these values for others consumption of silicon and lead are considered constant even if they may change during the years since it is unknown how they will change.

Finally and in order to calculate the "Pctg of world GDP invested in solar energy", the global investment made in solar energy in 2013 is collected from the Figure 44, which belongs to the article "*Renewables 2014 Global Status Report*" (2014) made by REN21 (Renewable Energy Policy Network for the 21st Century).

This global investment in solar power is:



Investment in solar = 74.8 + 38.9 = 113.7 Billion US\$

Figure 44. Global new investment in renewable energy by technology (2013). Source: REN21, 2014, "Renewables 2014 Global Status Report".

This investment is divided by the world GDP of this year (75 593 billion US\$), obtaining the fraction of world GDP that was invested in solar energy in 2013 (0.150411% in percentage). The value of this percentage is actually variable over the years but in the model it is used as a constant to simplify.



6.3 Causal Loop Diagram

Causal Loop Diagrams are an easy way to see and understand the relationships between variables in the system, and particularly to visualize the existing balancing or reinforcing loops.



Figure 45. Detailed Causal Loop Diagram of the system.

This Causal Loop Diagram (Figure 45) is much more detailed than the basic one presented at the beginning of section 6 (Figure 18), but it still does not contain all the elements of the model. It only shows the variables needed to understand the behavior of the system.

As in the basic CLD, most of the elements in this detailed CLD and the other CLDs coming up next have two material or technology dimensions: silicon and perovskite lead.



For that reason, there are again some black arrows meaning that their polarity can change or that it is not clearly defined as it comes from a comparison between the same elements of each material or technology. The polarity displayed in all these black arrows is the most expected or probable one.

Some loops are not easy to visualize in the detailed CLD (Figure 45), so the next figures (Figures 46 to 51) show every loop in a more comprehensible way. The reinforcing loops R1 and R2 are the same that in the basic CLD (Figure 18) but with more elements.



Figure 46. Reinforcing Loops R1, R2 and R3.

On one hand, there are three reinforcing loops (R1, R2 and R3) that dominate the behavior of the system (Figure 46). More investments allow to grow the capacity and so material needs are bigger. Then, both extraction and recycling rates increase and the costs of extracting and recycling decrease because of the learning and technical improvements. Finally, as PV production costs decrease, governments decide to invest more in solar energy and the reinforcing loops start again.

On the other hand, these reinforcing loops are also countered by two important balancing loops (B1 and B2) shown in Figure 47. These loops are very similar to the three reinforcing loops



seen above but the relation between the recycling rate and the extraction rate makes these loops balancing. A higher recycling rate reduces the extraction rate and then the cost of extracting is higher because there is less learning. As a result, the high costs bring down the investments, then the solar capacity is lower and the material needs and use decrease.



Figure 47. Balancing Loop B1 and B2.

Nevertheless, the reinforcing loops R1, R2 and R3 dominate over these two balancing loops B1 and B2. The system behavior is a progressive increase of the investments in solar, its capacity and the use of materials.



Figure 48. Reinforcing Loop R4.



Two other smaller reinforcing loops are R4 and R5 (Figure 48 and 49, respectively). These loops influence the recycling fraction for each material of the two dimensions. The loop R4 reduces the cost of recycling when the recycling rate rises and so the fraction of recycling increases making the recycling rate rising again.



Figure 49. Reinforcing Loop R5.

The loop R5 also reinforces the fraction of recycling by a rise in the recycling rate but with a different path. When the recycling rate rises, the extraction rate becomes lower and then the cost of extraction grows. This growth in the cost of extraction makes more interesting to recycle so that the fraction of recycling increases too.

Finally, there are two small balancing loops presented in Figure 50 and Figure 51 (B3 and B4, correspondingly), which simply balance a stock with its outflow. For example, in the loop B4 the higher is the total solar capacity the higher is the capacity that is scrapped, reducing so the total solar capacity.



Figure 51. Balancing Loop B4.



6.4 Model validation

The validation of the model is done by reaching a roughly behavior replication of a real reference mode.

In this system, the reference mode are the two variables "Total Investments in solar energy" and "Total Solar Capacity" at a global level from the year 2004 to 2013. In the Table 8 and Table 9 are presented, respectively, the historical annual values for the reference mode of each variable.

REF MODE Total Investments in solar energy		
Year	Billion US\$	
2004	12.1	
2005	16.3	
2006	21.7	
2007	38.7	
2008	59.5	
2009	62.9	
2010	100.3	
2011	157.8	
2012	142.9	
2013	113.7	

Table 8. New Global Total Investments in solar energy (2004-2013).Data source: UNEP, 2014, "Global Trends in Renewable Energy Investment 2014".

Table 9. World Total Solar Capacity (2004-2013).Data source: REN21, 2014, "Renewables 2014 Global Status Report".

REF MODE World Total Solar Capacity		
Year	Capacity (GW)	
2004	3.7	
2005	5.1	
2006	7.0	
2007	9.0	
2008	16.0	
2009	23.0	
2010	40.0	
2011	70.0	
2012	100.0	
2013	139.0	

Data for the annual total investments in solar energy in the world is collected from the report "*Global Trends in Renewable Energy Investment 2014*" made by the Frankfurt School-UNEP Centre. On the other hand, the values for the accumulated world total solar capacity are taken from the article "*Renewables 2014 Global Status Report*" made by REN21.



The next two graphs in Figure 52 and Figure 53 show how the built model approximately replicates, correspondingly, the historical evolution of the total investments in solar energy and the total solar capacity in the world from 2004 to 2013.



Figure 52. Replication of the Total Investments in solar energy.

In both graphs, the reference mode is represented in blue (number 1) while the simulated behavior is in red (number 2).



Figure 53. Replication of the Total Solar Capacity.

As it can be observed in the graphs, the achieved replications are not completely accurate. However, the model can be considered as valid enough since the shape of the simulated behavior is quiet similar to the historical behavior.



Lastly, it is important to comment all the changes done from the model replicating the reference mode to the model simulating the future. These modifications made to adapt the model for a simulation in a long term are:

- In the "Run Specs", the length of simulation is changed from 2004-2013 to 2004-2050.
- For the model replicating the reference mode, the lifetime of perovskite solar cells has an initial value of 5 years because the long-term stability is not still solved in 2013. In the model simulating until 2050, the initial value for the lifetime of perovskite cells is 22 years since it is assumed that it will improve in the coming years and stability will be guaranteed at least over 20 years. This assumption is explained in the section 5.1.
- In the same way, the model replicating the historical behavior uses an efficiency of perovskite solar cells of 20.1%, that is the record achieved nowadays. For the model simulating the future, it is estimated a power conversion efficiency of 40% as initial value for the slider. This assumption is also explained in the section 5.1.



6.5 Future estimations for the model

Once the built model roughly reproduces the reference mode from 2004 to 2013, some variables require future estimations for the model simulation until the year 2050.

To begin with, the world GDP is supposed to keep increasing with more or less the same tendency than in the last decade. Figure 54 shows the projection made for the world GDP with an average annual growth of 3%. This estimation of the annual growth for the world GDP is based on the recent report "*The World in 2050*" (February 2015) made by the multinational PwC (*PricewaterhouseCoopers*), one of the Big Four auditors. This large company affirms to "*project the world economy to grow at an average of just over 3% per annum in the period* 2014 - 2050".



Figure 54. Estimation for world GDP (billion US\$, constant 2005).

The estimations made for the future evolution for the cost of fossil fuels and the basic cost of solar energy until 2050 are shown in Figure 55.

Note that the cost of solar energy is then adjusted in the model by the variable "Adjustment in cost of solar energy", which is already explained in the section 6.1. As lot of experts affirm, it is assumed that solar energy will become cheaper than fossil fuels soon. This evolution is necessary for solar to become the first energy source in the world.

As it is defined in the section 6.2, these costs are named levelized cost of electricity (LCOE) and their units used are US\$ per megawatt-hour.



The estimations for the levelized cost of fossil fuels are based on experts from the *German Institute for Economic Research* (DIW Berlin), who have projected in the article "*Current and Prospective Costs of Electricity Generation until 2050*" (2013) that the cost of fossil fuels will be more or less constant until 2050, for a constant value of money. Other experts from the *Fraunhofer Institute for Solar Energy Systems* (Fraunhofer ISE) declare that there will be a small increase on the cost of fossil fuels between the years 2020 and 2030.

Moreover, also experts from the *Fraunhofer ISE* affirm in their study "*Levelized Cost Of Electricity of Renewable Energy Technologies*" (2013) that the cost of solar energy in 2050 will be reduced around 60% from the cost in 2013. This decreasing evolution for solar cost is very expected since the future improvements in both the new and conventional technologies will obviously make their production costs cheaper.



Figure 55. Estimation for costs of fossil fuels and solar energy.

Other sources used to contrast all these estimations are the report "Levelized Cost and Levelized Avoided Cost of New Generation Resources in the Annual Energy Outlook 2014" made by the U.S. Energy Information Administration (EIA) and the recent study "Current and Future Cost of Photovoltaics" (February 2015) by Agora Energiewende.

Finally, the last future estimation is for the power conversion efficiency (PCE) of silicon solar cells (Figure 56). Some experts say that the efficiency of silicon cells is close to reach its limit due to a problem of capability. In consequence, it estimated a small annual growth for this efficiency but each year more slowly. A small future increase is still assumed since there will also be some improvements in the silicon technology even if the perovskite technology becomes more efficient.



Figure 56. Estimation for the PCE of silicon solar cells.

It is also important to point out that, as it is explained in the section 6.2, this estimated PCE of silicon cells is an approximate average of all the silicon solar cells commercialized in the future, proportionally to the market share of each type of silicon cell.



7. RESULTS

The dynamic model can be simulated in different scenarios through five sliders that allow the user to modify the value of five constants (Figure 57). These constants are:

- "Scenario effect on investments": a multiplier for the total investments to simulate a lower or higher investment policy.
- "Estimated Efficiency of Perovskite solar cells": the power conversion efficiency that is estimated to be reached in the coming years for commercial perovskite solar cells.
- "Lifetime Perovskite cells": the average lifespan that is estimated to be achieved in the coming years for commercial perovskite solar cells.
- "Received Sunlight energy": the average sunlight energy received by the solar panels in the Earth's surface.
- "Parameter alpha for logistics function": the parameter that determines the sensibility of the logistic function used in the investment share for each technology. The higher is this parameter, the more sensible is the function.



Figure 57. Sliders for the model simulation.



The initial values for these five constants are the ones set in the Figure 57, the same that are already shown in the Table 7 of section 6.2.2.

In the next sections 7.1, 7.2 and 7.3 the system is simulated in a moderate scenario, pessimistic scenario and optimistic scenarios, respectively.

Note that only the constants "Scenario effect on investments", "Estimated Efficiency of Perovskite solar cells" and "Lifetime Perovskite cells" are modified in the next three simulated scenarios because just these three constants have a considerable influence on the results of the simulation and they have more probabilities to be different in the real future. Even so, the constants "Received Sunlight energy" and "Parameter alpha for the logistic function" are defined as sliders in case that the user of the model wants to change these parameters in an easy way for future simulations.



7.1 Scenario 0: Moderate scenario

In this moderate scenario the values in the sliders are not modified. This means that all the constants have their initial values in this first simulation from 2004 to 2050:

- "Scenario effect on investments" = 1
- "Estimated Efficiency of Perovskite solar cells" = 40%
- "Lifetime Perovskite cells" = 22

First, it is checked how the world total solar capacity grows and becomes an important source of energy in the future (Figure 58). It is important to confirm this behavior because one the main assumptions for this model is that solar energy becomes one of the leading sources of energy in the coming decades. Otherwise, it would not be interesting to carry out the analysis for the problems of this study.



Figure 58. Scenario 0: Total Solar Capacity.

In 2050 this global capacity would be of 1418 gigawatts, which is more than ten times the current solar capacity in the world. This value is still far to be enough to satisfy the majority of the world's energy consumption but the solar development would be going in the right direction and it could be considered as one of the predominant sources of energy in the world.

In the next figure (Figure 59) it can be observed that most of the new solar capacity developed in the next decades would come from the photovoltaic technology using perovskite.

The production of silicon solar cells would start to decrease slowly from the year 2030. In terms of capacity (gigawatts/year), perovskite solar cells production would be twelve times bigger than for silicon solar cells in 2050.





Figure 59. Scenario 0: Capacity per Technology.

This fact is important because it shows that, as it was expected, the perovskite technology would become dominant in photovoltaics. This is the consequence of higher investments in the development of perovskite technology than in the extension of silicon solar cells production, as it shown in the Figure 60.



Figure 60. Scenario 0: Total Investments in solar energy and Investments per Technology.

Obviously, the total investments in solar energy would increase on the same way that the solar capacity because capacity grows due to an increase on the investments. Around 88% of the total investments in solar in the year 2050 would be put in the perovskite technology, while the other 12% would be for the traditional silicon one.

This investment share in photovoltaic technologies can be also observed in the Figure 61.





Figure 61. Scenario 0: Investment Share per Technology.

The growth of perovskite technology would have a considerable effect on the estimated cost of solar energy. As shown in Figure 62, the adjustment due to the development of cheap perovskite solar cells would reduce the global cost of solar energy to almost half of the estimated cost in 2050.



Figure 62. Scenario 0: Adjustment in cost of solar energy.

Even if perovskite cells would become predominant over silicon cells, the required materials for both have to be analyzed. In the next two figures they are shown the accumulated quantities produced and recycled both for silicon and lead together with their fraction of recycling (Figure 63 and Figure 64, respectively).

Produced and recycled silicon would logically increase because these stocks are cumulative, they do not have outflows. However, their increase would be relatively slow compared to lead.





Figure 63. Scenario 0: Produced, recycled and fraction of recycling silicon.

The recycled quantity of silicon would be slightly higher than the new produced silicon, which is the silicon coming from extraction. This happens because the fraction recycling for silicon is over 0.5. This fraction is almost constant during the whole simulation, it would only grow a bit and its value is around 0.6.

In the length of the simulation, the produced silicon would be still extremely small compared to the silicon resources in the world, specifically the abundant quartz minerals required to produce the high pure silicon for solar cells.

Therefore, it could be affirmed that there would not be problems of scarcity for silicon in a very long term.



Figure 64. Scenario 0: Produced, recycled and fraction of recycling lead.



Lead production and recycling quantities would become much bigger than for silicon. This fact would happen not only because the perovskite technology would become predominant, but also because the annual consumption of lead in other sectors is more than five times the annual consumption of silicon in other sectors.

In this case, the new produced lead would be bigger than the recycled one since the recycling fraction for lead is under 0.5. Furthermore, the fraction of recycling for lead would decrease from around 0.37 in 2004 to around 0.28 in 2050.

According to *Asian Metal*, the current proven resource volume of lead in the world is more than 2 billion tons and the reserve volume is about 89 million tons. This means that in the simulation the current reserves of lead would be finish in the year 2021. Lead proven resources would still be enough for several decades with the simulated consumption but still this material could be consider as soon exhaustible.

To address this potential problem of lead scarcity in the future, it should be recycled a much bigger fraction of lead than the fraction obtained in this simulation. Huge efforts in lead recycling would need to be done if it is desired to continue with its use in the future.



Figure 65. Scenario 0: Lead consumed in solar vs. lead consumed in other sectors.

Finally, lead consumption for photovoltaics would be negligible compared to the world consumption in other sectors. Figure 65 shows how inappreciable would be the use of lead to produce the increasing amount of perovskite solar cells in the future. Therefore, the last problem concerning the environmental impact of lead in perovskite cells production could be considered insignificant.

All the results obtained in this first simulation are then contrasted with a pessimistic scenario and an optimistic scenario in the next sections 7.2 and 7.3, respectively.



7.2 Scenario 1: Pessimistic scenario

Then, the system is simulated in a pessimistic scenario with a lower investment policy in photovoltaics, a lower estimated efficiency and a lower lifetime for perovskite solar cells. The values for the three constants defining this scenario are:

- "Scenario effect on investments" = 0.5
- "Estimated Efficiency of Perovskite solar cells" = 25%
- "Lifetime Perovskite cells" = 20

With the first of these constants, the investments in solar would be half than in the moderate scenario. In this case, perovskite technology would not develop as expected and the PCE would just be around 25%, which is the record efficiency of current silicon cells. The average lifetime for perovskite solar cells would be of 20 years, which is the minimum required to be attractive in the PV market.



Figure 66. Scenario 1: Total Solar Capacity.

As in the previous scenario, the first step is checking how photovoltaics would grow in the coming decades. Figure 66 shows that in this pessimistic scenario the total solar capacity would increase much less than in the moderate one.

This world capacity would be around 670 gigawatts in 2050, which is less than the half than in the previous scenario and would make photovoltaics grow much slower in its race to become a predominant source of energy in the world.

The smaller capacity is due to a huge reduction on the total investments in solar energy, as it is observed in the Figure 68, which is caused by the low investment policy set for this pessimistic scenario.





Figure 67. Scenario 1: Capacity per Technology.

Nevertheless, most of the new capacity build in the next years would come again from perovskite solar cells. Figure 67, Figure 68 and Figure 69 show how the perovskite technology would still become predominant over the traditional silicon one, even if perovskite cells would not be develop as much as expected.

With a PCE of 25% and a lifetime of 20 years, perovskite solar cells would have slightly worst properties than silicon cells in the future. However, their price would be considerably smaller than for silicon solar cells since they would be much cheaper to manufacture. This is the main reason why the investment share and built capacity should be also focused in perovskite technology in a pessimistic scenario.



Figure 68. Scenario 1: Total Investments in solar energy and Investments per Technology.





Figure 69. Scenario 1: Investment Share per Technology.

The adjustment made in the global cost of solar energy (Figure 70) would be almost the same than in the previous scenario. As the perovskite technology is again the most developed in this simulation, the cost of solar energy would be amply adjusted because of the lower costs of perovskite cells.



Figure 70. Scenario 1: Adjustment in cost of solar energy.

Regarding to the accumulated production and recycling of both silicon and lead (Figure 71 and Figure 72, respectively), the system behavior in this simulation would be practically identical to the obtained in the moderate scenario.

Even if the photovoltaic production would be much smaller in this scenario, the use of materials would vary virtually nothing compared to the previous simulation. This fact is attributable to


the minor fraction that would represent the materials consumed for solar cells production over the global consumptions in other sectors.



Figure 71. Scenario 1: Produced, recycled and fraction of recycling silicon.

Obviously, as the cumulative produced and recycled materials would not have changed almost nothing, the fraction of recycling for each material would also be practically identical to the simulated in the moderate scenario.



Figure 72. Scenario 1: Produced, recycled and fraction of recycling lead.

Lead would also have scarcity problems in the future for this scenario and it should be necessary again to highly rise its fraction of recycling.

It is then possible to affirm that, in this case, the behavior of the material production and recycling is scarcely influenced by the consumption in the photovoltaic market.



The last graph (Figure 73) shows that, as it could be anticipated, the annual lead consumption for perovskite solar cells production would be insignificant compared to the global consumption of lead in other sectors. This fact already happens in the moderate scenario so it is logical that it also happens in this case where the manufacture of perovskite cells is smaller. Then, the concern about the environmental impact of lead could be not considerate once again in perovskite solar cells production.



Figure 73. Scenario 1: Lead consumed in solar vs. lead consumed in other sectors.

The only remark in comparison with the moderate scenario is that the total investments in solar energy and so its global capacity are considerably smaller, but this does not really affect all the other results.



7.3 Scenario 2: Optimistic scenario

Finally, the system is simulated in an optimistic scenario with a higher investment policy in photovoltaics, a higher estimated efficiency and a higher lifetime for perovskite solar cells. The values for the three constants defining this optimistic scenario are:

- "Scenario effect on investments" = 1.5
- "Estimated Efficiency of Perovskite solar cells" = 50%
- "Lifetime Perovskite cells" = 25

The first scenario effect would make total investments in solar energy a 50% bigger than in the moderate scenario and three times bigger than in the pessimistic one. Then, the perovskite technology would be more developed and perovskite solar cells would reach a power conversion efficiencies of 50% and an average lifetime of 25 years.



Figure 74. Scenario 2: Total Solar Capacity.

One more time, the first verification is about the growth of photovoltaics. Figure 74 shows how fast the world total solar capacity would rise in this optimistic scenario, reaching 2459 gigawatts in 2050. If this situation is reproduced in the future, photovoltaics would rapidly become one of the main source of energy in the world.

As in the two previous scenarios, the predominant photovoltaic technology would be the one using perovskite (Figure 75). Both silicon and perovskite technologies would have an annual growth much higher in this scenario.

However and like in the other scenarios, the new capacity for silicon cells would start decreasing from 2030 because of a reduction in the annual investments for this technology from this year (Figure 76).





Figure 75. Scenario 2: Capacity per Technology.

It is logical that there would be a huge dominance of perovskite technology in the future because in this optimistic simulation the perovskite cells would have the same lifetime than silicon cells but with almost the double power conversion efficiency and much cheaper production costs.



Figure 76. Scenario 2: Total Investments in solar energy and Investments per Technology.

In the same way observed in the simulation, with these properties for perovskite solar cells the investments made in solar and specifically in the perovskite technology should be very significant. Figure 76 and Figure 77 show this behavior.

Governments should then progressively and highly increase the annual investments in photovoltaics if it is found in the future that perovskite technology is developing in a great way.





Figure 77. Scenario 2: Investment Share per Technology.

Once again, the behavior for the adjustment in the estimated cost of solar energy (Figure 78) does not vary a lot from the obtained in the moderate scenario.

The adjusted cost of solar energy would again reduce the estimated cost to almost its half in the year 2050, due to the dominance of the cheap perovskite technology.



Figure 78. Scenario 2: Adjustment in cost of solar energy.

In respect of the cumulative produced and recycled materials and their recycling fraction (Figure 79 and Figure 80), the simulated behavior is once more almost identical to the moderate and pessimistic scenarios.





Figure 79. Scenario 2: Produced, recycled and fraction of recycling silicon.

So, as in the previous simulations, there would not be problems with the abundant resources of silicon or quartz minerals but it still seems that there would be possible problems of scarcity for lead in the future.



Figure 80. Scenario 2: Produced, recycled and fraction of recycling lead.

Finally and like in the other scenarios, the environmental impact of the lead used in perovskite solar cells could be ignored.

Even in this optimistic situation where the perovskite solar cells production would be bigger, the use of lead to manufacture these cells would be extremely small compared to the global 8 million tons consumed in average per year in other sectors (Figure 81).





Figure 81. Scenario 2: Lead consumed in solar vs. lead consumed in other sectors.

Summing up, there are not notable differences between the results of the moderate, the pessimistic and the optimistic scenarios. Therefore, it can be considered that the general results of the system simulation are sufficiently valid, since they do not vary significantly with big changes in the investment policy and in the estimations concerning the promising perovskite technology for photovoltaics.

Most of the obtained results validate the hypothesis made in the section 5.1. The first validation is that, in the next decades, photovoltaics would considerably grow in the right direction to become one of the main energy sources in the world.

Then it is found that lead would have a potential problem of scarcity in the future, as it was expected. Nonetheless, it has to be pointed out that this problem does not come from lead use in photovoltaics because it would be really small compared with its global annual consumption in other sectors.

For the same reason, the hypothesis about the environmental impact of lead due to the perovskite solar cells production is also validated since it would be insignificant compared to other lead consumptions.

However, the hypothesis about recycling is rejected. The fraction of recycling for lead would not be as high as it should, and it would actually decrease over time instead of increasing. Measures and actions would need to be carried out in order to rise the recycling fraction of lead to its maximum.



8. CONCLUSIONS

In the results of the three moderate, pessimistic and optimistic scenarios simulated in this paper there are not evidences of most of the problems contemplated for the development of photovoltaics until the year 2050 and it seems that until a longer term.

In consequence, it would be advisable to set a strong investment policy for renewable solar energy in order to develop PV technologies and the global solar capacity as much as possible. With higher investments, the improvements would be more important so that the lifetime and efficiency of perovskite solar cells could increase further.

As it was supposed, perovskite technology should become predominant in photovoltaics. Therefore, governments should decide to invest a much bigger proportion in the development of this now promising technology instead of building more and more purifying installations to increase the production of monocrystalline and polycrystalline silicon for traditional silicon solar cells.

Even if the major concern about the environmental impact of lead use in perovskite solar cells has been finally considered as irrelevant, the results of this study demonstrate that there is a potential problem of scarcity for lead.

This issue requires of a policy that strongly increases the current fraction of recycling for this material if it is desired to keep using it. Furthermore, lead use in perovskite solar cells is really minor compared to other consumptions in the world. Other sectors with high lead consumption should therefore make also big efforts in recycling this material instead of using the lead coming from new extraction.

In the photovoltaic sector there is already a possible solution to substitute the use lead in perovskite solar cells with another material. This alternative material for the production of cheap high-effective perovskite layers is tin (Sn). Moreover, this solution would also end with the concerns about the environmental impact of lead. Nonetheless, researches and improvements are still far from producing perovskite layers with tin as effective as with lead.

It should be pointed out that two-level solar cells combining silicon and perovskite layers could be a prominent option for the future of photovoltaics. The name of these compounds is tandem solar cells and there are already some current researches for their development.

After the analysis done, this combined cells seem attractive since silicon resources are extremely abundant and it does not have scarcity problems. However, the required pure silicon would still be expensive to manufacture. In consequence, these tandem solar cells would only be really interesting in the future if they achieve much higher power conversion efficiencies than one-level perovskite solar cells.



To finish off, it is worth mentioning that the system dynamic model built in this study could be simply adjusted to analyze other materials used in photovoltaics. For example, it could be useful in case that it is found a suspected scarcity for any other of the materials which make up a solar cell.



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APPENDIX A: The dynamic model





APPENDIX B: The equations

PEROVSKITE_LEAD_in_use(t) = PEROVSKITE_LEAD_in_use(t - dt) + (PEROVSKITE_LEAD_new_for_Solar - PEROVSKITE_LEAD_used) * dt

```
INIT PEROVSKITE_LEAD_in_use = 0
```

INFLOWS:

PEROVSKITE_LEAD_new_for_Solar = (PEROVSKITE_LEAD_Needs*PEROVSKITE_LEAD_density)/Unit_converter_2

OUTFLOWS:

PEROVSKITE_LEAD_used = PEROVSKITE_LEAD_in_use/Lifetime_PEROVSKITE_cells

 $\square Produced_LEAD(t) = Produced_LEAD(t - dt) + (Extraction_rate_LEAD) * dt$

```
INIT Produced_LEAD = 0
```

INFLOWS:

Extraction_rate_LEAD = PEROVSKITE_LEAD_new_for_Solar+Other_LEAD_consumption-Recycling_rate_LEAD

```
\square Produced\_SILICON(t) = Produced\_SILICON(t - dt) + (Extraction\_rate\_SILICON) * dt
```

```
INIT Produced_SILICON = 0
```

INFLOWS:

Extraction_rate_SILICON = SILICON_new_for_Solar+Other_SILICON_consumption-Recycling_rate_SILICON

```
\square Recycled\_LEAD(t) = Recycled\_LEAD(t - dt) + (Recycling\_rate\_LEAD) * dt
```

```
INIT Recycled_LEAD = 0
```

INFLOWS:

Recycling_rate_LEAD = (PEROVSKITE_LEAD_used+Other_LEAD_consumption)*Fraction_recycling_LEAD

 $\square Recycled_SILICON(t) = Recycled_SILICON(t - dt) + (Recycling_rate_SILICON) * dt$

INIT Recycled_SILICON = 0

INFLOWS:

Recycling_rate_SILICON = (SILICON_used+Other_SILICON_consumption)*Fraction_recycling_SILICON

□ SILICON_in_use(t) = SILICON_in_use(t - dt) + (SILICON_new_for_Solar - SILICON_used) * dt



INIT SILICON_in_use = 0

INFLOWS:

SILICON_new_for_Solar =
(SILICON_Needs*SILICON_density)/Unit_converter_2

OUTFLOWS:

SILICON_used = SILICON_in_use/Lifetime_SILICON_cells

Total_Solar_Capacity(t) = Total_Solar_Capacity(t - dt) + (New_capacity -Scrapped_capacity) * dt

INIT Total_Solar_Capacity = 3.7

INFLOWS:

New_capacity = Capacity_per_Technology[WithSilicon]+Capacity_per_Technology[WithPerovskite]

OUTFLOWS:

Scrapped_capacity = Total_Solar_Capacity/Lifetime_solar_cells

• Adjusted_Cost_of_solar_energy =

(Cost_of_solar_energy*Investment_Share_per_Technology[WithSilicon]*Adjustment_in_cost_of_solar_energy[WithSilicon])

+

(Cost_of_solar_energy*Investment_Share_per_Technology[WithPerovskite]*Adjustment_in _cost_of_solar_energy[WithPerovskite])

• Adjustment_in_cost_of_solar_energy[WithSilicon] = 1

• Adjustment_in_cost_of_solar_energy[WithPerovskite] =

 $(Cost_of_extracting_and_processing_LEAD*(1-$

Fraction_recycling_LEAD)+Cost_of_recycling_LEAD*Fraction_recycling_LEAD)/(Cost_of _extracting_and_processing_SILICON*(1-

Fraction_recycling_SILICON)+Cost_of_recycling_SILICON*Fraction_recycling_SILICON)

Ø

Capacity_per_Technology[Technology] = GRAPH(Investments_per_Technology[Technology]*(1+Efficiency_of_solar_cells[Technolo gy]))



335), (2929, 337), (2980, 338), (3030, 341), (3081, 343), (3131, 346), (3182, 348), (3232, 349), (3283, 351), (3333, 354), (3384, 356), (3434, 359), (3485, 360), (3535, 362), (3586, 363), (3636, 367), (3687, 367), (3737, 368), (3788, 371), (3838, 373), (3889, 375), (3939, 376), (3990, 376), (4040, 379), (4091, 381), (4141, 381), (4192, 383), (4242, 383), (4293, 384), (4343, 386), (4394, 386), (4444, 387), (4495, 387), (4545, 389), (4596, 390), (4646, 390), (4697, 394), (4747, 394), (4798, 395), (4848, 395), (4899, 397), (4949, 398), (5000, 400)

O Converted_electrical_energy[Technology] = Received_sunlight_energy*Efficiency_of_solar_cells[Technology]

 \bigotimes Cost of extracting and processing LEAD = GRAPH(Produced LEAD)

(0.00, 8.13), (20.8, 6.83), (41.7, 6.03), (62.5, 5.34), (83.3, 4.90), (104, 4.66), (125, 4.46), (146, 4.22), (167, 3.92), (188, 3.68), (208, 3.48), (229, 3.34), (250, 3.24), (271, 3.11), (292, 3.01), (313, 2.94), (333, 2.91), (354, 2.87), (375, 2.87), (396, 2.87), (417, 2.87), (438, 2.91), (458, 3.01), (479, 3.04), (500, 3.21)

Cost_of_extracting_and_processing_SILICON = GRAPH(Produced_SILICON)

(0.00, 7.40), (20.8, 7.30), (41.7, 7.23), (62.5, 7.13), (83.3, 7.03), (104, 6.93), (125, 6.89), (146, 6.86), (167, 6.79), (188, 6.76), (208, 6.72), (229, 6.66), (250, 6.62), (271, 6.55), (292, 6.52), (313, 6.49), (333, 6.49), (354, 6.49), (375, 6.49), (396, 6.45), (417, 6.49), (438, 6.49), (458, 6.49), (479, 6.55), (500, 6.66)

Ø

0

Cost_of_fossil_fuels = GRAPH(TIME)

(2004, 162), (2005, 173), (2006, 183), (2007, 198), (2008, 191), (2009, 187), (2010, 180), (2011, 183), (2012, 180), (2013, 176), (2014, 172), (2015, 169), (2016, 166), (2017, 165), (2018, 166), (2019, 168), (2020, 169), (2021, 172), (2022, 175), (2023, 177), (2024, 179), (2025, 181), (2026, 183), (2027, 184), (2028, 185), (2029, 186), (2030, 187), (2031, 186), (2032, 185), (2033, 184), (2034, 183), (2035, 183), (2036, 183), (2037, 183), (2038, 183), (2039, 183), (2040, 183), (2041, 182), (2042, 182), (2043, 181), (2044, 181), (2045, 180), (2046, 180), (2047, 180), (2048, 179), (2049, 179), (2050, 179)

Output Cost_of_recycling_LEAD = GRAPH(Recycled_LEAD)

(0.00, 8.41), (26.3, 6.92), (52.6, 6.10), (78.9, 5.71), (105, 5.46), (132, 5.30), (158, 5.14), (184, 5.02), (211, 4.89), (237, 4.83), (263, 4.73), (289, 4.70), (316, 4.67), (342, 4.63), (368, 4.63), (395, 4.63), (421, 4.60), (447, 4.60), (474, 4.60), (500, 4.57)

Ø

Cost_of_recycling_SILICON = GRAPH(Recycled_SILICON)

(0.00, 8.89), (26.3, 8.06), (52.6, 7.56), (78.9, 7.17), (105, 6.95), (132, 6.79), (158, 6.63), (184, 6.51), (211, 6.44), (237, 6.35), (263, 6.29), (289, 6.19), (316, 6.16), (342, 6.10), (368, 6.10), (395, 6.10), (421, 6.03), (447, 6.00), (474, 6.00), (500, 5.97)



Cost_of_solar_energy = GRAPH(TIME)

Ø

(2004, 576), (2005, 540), (2006, 558), (2007, 504), (2008, 450), (2009, 378), (2010, 324), (2011, 288), (2012, 252), (2013, 216), (2014, 198), (2015, 184), (2016, 170), (2017, 160), (2018, 151), (2019, 143), (2020, 138), (2021, 133), (2022, 129), (2023, 125), (2024, 122), (2025, 118), (2026, 117), (2027, 115), (2028, 113), (2029, 111), (2030, 109), (2031, 108), (2032, 107), (2033, 106), (2034, 105), (2035, 104), (2036, 103), (2037, 102), (2038, 102), (2039, 101), (2040, 101), (2041, 100), (2042, 100), (2043, 99.0), (2044, 99.0), (2045, 99.0), (2046, 98.0), (2047, 98.0), (2048, 98.0), (2049, 97.0), (2050, 97.0)

• Efficiency_of_solar_cells[WithSilicon] = Efficieny_of_Silicon_solar_cells/100

• Efficiency_of_solar_cells[WithPerovskite] = Estimated_Efficiency_of_Perovskite_solar_cells/100

Ø
Efficieny_of_SILICON_solar_cells = GRAPH(TIME)

(2004, 15.0), (2005, 15.5), (2006, 16.1), (2007, 16.7), (2008, 17.4), (2009, 18.2), (2010, 19.0), (2011, 19.9), (2012, 20.9), (2013, 22.0), (2014, 22.7), (2015, 23.3), (2016, 23.9), (2017, 24.4), (2018, 24.9), (2019, 25.3), (2020, 25.7), (2021, 26.0), (2022, 26.3), (2023, 26.5), (2024, 26.7), (2025, 26.8), (2026, 26.9), (2027, 27.0), (2028, 27.1), (2029, 27.2), (2030, 27.3), (2031, 27.4), (2032, 27.5), (2033, 27.6), (2034, 27.7), (2035, 27.8), (2036, 27.9), (2037, 28.0), (2038, 28.1), (2039, 28.2), (2040, 28.3), (2041, 28.4), (2042, 28.5), (2043, 28.6), (2044, 28.7), (2045, 28.8), (2046, 28.9), (2047, 29.0), (2048, 29.1), (2049, 29.2), (2050, 29.3)

• Estimated_Efficiency_of_PEROVSKITE_solar_cells = 40

Fraction_recycling_LEAD =

GRAPH(Cost_of_extracting_and_processing_LEAD/Cost_of_recycling_LEAD)

(0.00, 0.00), (0.0513, 0.054), (0.103, 0.0889), (0.154, 0.124), (0.205, 0.146), (0.256, 0.168), (0.308, 0.187), (0.359, 0.206), (0.41, 0.219), (0.462, 0.235), (0.513, 0.251), (0.564, 0.27), (0.615, 0.286), (0.667, 0.302), (0.718, 0.314), (0.769, 0.324), (0.821, 0.337), (0.872, 0.349), (0.923, 0.359), (0.974, 0.368), (1.03, 0.381), (1.08, 0.39), (1.13, 0.403), (1.18, 0.413), (1.23, 0.422), (1.28, 0.432), (1.33, 0.441), (1.38, 0.454), (1.44, 0.467), (1.49, 0.486), (1.54, 0.502), (1.59, 0.517), (1.64, 0.537), (1.69, 0.562), (1.74, 0.594), (1.79, 0.625), (1.85, 0.679), (1.90, 0.778), (1.95, 0.873), (2.00, 0.997)

Ø

Fraction_recycling_SILICON =

GRAPH(Cost_of_extracting_and_processing_SILICON/Cost_of_recycling_SILICON)

(0.00, 0.00), (0.0513, 0.0921), (0.103, 0.149), (0.154, 0.203), (0.205, 0.248), (0.256, 0.302), (0.308, 0.343), (0.359, 0.384), (0.41, 0.416), (0.462, 0.444), (0.513, 0.473), (0.564, 0.502), (0.615, 0.521), (0.667, 0.537), (0.718, 0.549), (0.769, 0.562), (0.821, 0.575), (0.872, 0.581), (0.923, 0.59), (0.974, 0.597), (1.03, 0.606), (1.08, 0.616), (1.13, 0.622), (1.18, 0.635), (1.23, 0.592), (0.974, 0.597), (0.97



0.638), (1.28, 0.648), (1.33, 0.654), (1.38, 0.657), (1.44, 0.667), (1.49, 0.679), (1.54, 0.698), (1.59, 0.721), (1.64, 0.743), (1.69, 0.765), (1.74, 0.787), (1.79, 0.81), (1.85, 0.835), (1.90, 0.867), (1.95, 0.898), (2.00, 1.00)

Investments_per_Technology[Technology] =
 Total_Investments_in_solar_energy*Investment_Share_per_Technology[Technology]

○ Investment_Share_per_Technology[WithSilicon] = (EXP(-

Parameter_alpha__for_logistic_function*Cost_of_extracting_and_processing_SILICON))/((EXP(-

Parameter_alpha__for_logistic_function*Cost_of_extracting_and_processing_SILICON))+(EXP(-

 $Parameter_alpha_for_logistic_function*Cost_of_extracting_and_processing_LEAD)))$

○ Investment_Share_per_Technology[WithPerovskite] = (EXP(-

Parameter_alpha__for_logistic_function*Cost_of_extracting_and_processing_LEAD))/((EX P(-

Parameter_alpha__for_logistic_function*Cost_of_extracting_and_processing_SILICON))+(EXP(-

 $Parameter_alpha_for_logistic_function*Cost_of_extracting_and_processing_LEAD)))$

○ Lifetime_PEROVSKITE_cells = 22

• Lifetime_SILICON_cells = 25

• Lifetime_solar_cells =

Lifetime_SILICON_cells*Investment_Share_per_Technology[WithSilicon]+Lifetime_PERO VSKITE_cells*Investment_Share_per_Technology[WithPerovskite]

- \bigcirc Other_LEAD_consumption = 8
- Other_SILICON_consumption = 1.55
- \bigcirc Parameter_alpha_for_logistic_function = 0.5
- Pctg_of_world_GDP_invested_in_solar_energy = 0.150411

• PEROVSKITE_LEAD_density = 11340

• PEROVSKITE_LEAD_Needs =

(((Capacity_per_Technology[WithPerovskite]*Unit_converter_1)/Converted_electrical_ener gy[WithPerovskite])*Thickness_of_PEROVSKITE_LEAD_layers)/Waste_material_adjustm ent[WithPerovskite]

- \bigcirc Received_Sunlight_energy = 164
- \bigcirc Scenario_effect_on_investments = 1
- \bigcirc SILICON_density = 2329

• SILICON_Needs =

(((Capacity_per_Technology[WithSilicon]*Unit_converter_1)/Converted_electrical_energy[WithSilicon])*Thickness_of_SILICON_layers)/Waste_material_adjustment[WithSilicon]



• Thickness_of_PEROVSKITE_LEAD_layers = 500/1000000000

• Thickness_of_SILICON_layers = 100/1000000

• Total_Investments_in_solar_energy = Scenario_effect_on_investments*World_GDP*(Pctg_of_world_GDP_invested_in_solar_ene rgy/100)*(Cost_of_fossil_fuels/Adjusted_Cost_of_solar_energy)

• Unit_converter_1 = 100000000

• Unit_converter_2 = 1000000000

• Waste_material_adjustment[Technology] = (1-0.7)*(1-0.2)*(1-0.3)

 \bigcirc World_GDP = GRAPH(TIME)

(2004, 43412), (2005, 46965), (2006, 50880), (2007, 57328), (2008, 62858), (2009, 59539), (2010, 65217), (2011, 72140), (2012, 73514), (2013, 75593)