VIPERLAB

FULLY CONNECTED **VI**RTUAL AND **P**HYSICAL P**ER**OVSKITE PHOTOVOLTAICS **LAB**

D 10.2

DATABASE OF MATERIAL USAGE, ENERGY DEMAND AND PROCESS FLOWS

DELIVERABLE REPORT

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FULLY CONNECTED VIRTUAL AND PHYSICAL PEROVSKITE PHOTOVOLTAICS LAB VIPERLAB

DELIVERABLE

D 10.2 DATABASE OF MATERIAL USAGE, ENERGY DEMAND AND PROCESS FLOWS

Project References

Project Acronym	VIPERLAB
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Deliverable References

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1.4	Revised Final Draft	28/05/2024	CENER, HZB	A. Buceta, N. Maticiuc

DISCLAIMER

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N°101006715

‘Fully connected virtual and physical perovskite photovoltaics lab' VIPERLAB is a Collaborative Project funded by the European Commission under Horizon 2020. Contract: 101006715, Start date of Contract: 01/06/2021; Duration: 42 months.

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EXECUTIVE SUMMARY

VIPERLAB is an infrastructure project that aims to create a European environment, where various physical and virtual infrastructures from 13 VIPERLAB partners can be accessed by different users from Europe and abroad. VIPERLAB identifies perovskite PV as the key emerging technology that will be the lever for a future market penetration of EU-based PV production with lowest costs and lowest carbon footprint.

The overall goal of the work package 10 is to provide guidance for the infrastructure and technology development within VIPERLAB by evaluating and optimizing the environmental, social and economic impact of new perovskite-based technologies. To this end, this work package will:

- Provide the data (material, process flows etc.) necessary for such an evaluation.
- Evaluate the environmental (Life Cycle Assessment, LCA), social and economic (Levelized Cost of Electricity, LCOE) impact of new perovskite-based technologies and how this impact is affected by the application, device design, choice of equipment and process.

This report presents the results of the consultation with consortium members, bibliographic sources and material suppliers, on material and energy flow and cost data that will conform the life cycle inventory (LCI). All the collected data will be presented in a database that will be available on the VAPO platform, the ultimate purpose of which is to facilitate the subsequent life cycle and cost analysis to be carried out at a later stage. The steps followed to convert the Excel file, where all the data were collected, into a functional data base are also described in the report.

1. INTRODUCTION

The Life cycle assessment (LCA) is defined by the ISO 14040 as the compilation and evaluation of the inputs, outputs and the potential environmental impacts of a product system throughout its life cycle.[1]

LCA studies are gaining importance due to the growing interest in determining the environmental impact of products. For an LCA analysis, all stages of the product, from the extraction of raw materials, the manufacturing processes, through the product's lifetime, to its disposal, must be considered. As shown in Figure 1, the first step is to define the goal and scope of the study for the product or process, in this case it will be related to perovskite solar cells. The following step would be establishing the life cycle inventory (LCI)., To do so, it is essential to collect data for all process steps and the entire lifetime of the case study. This involves analysing inputs and outputs related to energy, materials, products, sub-products, waste, emissions, and other relevant factors. Once the inventory is ready, the data is associated to environmental impact categories and indicators, this phase is known as the life cycle impact assessment (LCIA). The last step is to analyse the LCI and LCIA results keeping in mind the uncertainty and accuracy of the data. By doing so, a thorough assessment of the environmental impact of the product, or process in question, is ensured.

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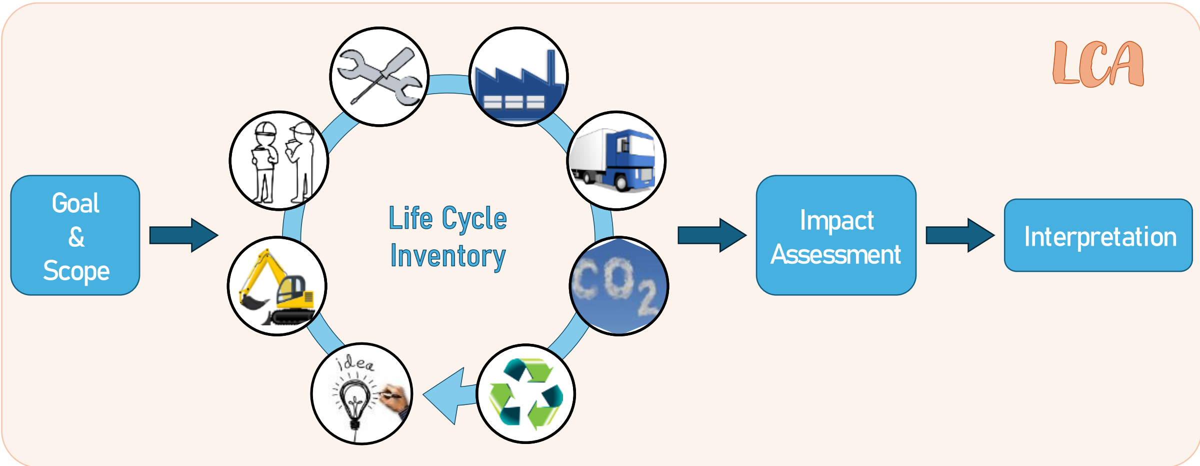

Figure 1. Schematic representation of LCA methodology phases (Source: Alicia Buceta, CENER).

In the previous deliverable (D.10.1) the key devices for perovskite solar cell were defined, therefore the scope and goal of the LCA will be single junction p-i-n and n-i-p configurations, and 2T and 4T tandem solar cells. Based on the selected key devices, and thanks to the support and expertise of the consortium, a list of the main materials used for the fabrication of these cells was drawn up. This list of materials and key devices represents the basis on which the LCI will be carried out. These deliverable details the steps followed to carry out part of the LCI, as well as its subsequent adaptation for the preparation of a database with the collected information.

2. DATA COLLECTION AND UNIFICATION

The scope of the LCA study are perovskite solar cells, and more precisely n-i-p and p-i-n configuration, and 2T and 4T tandem with crystalline silicon cells as the bottom cell. This deliverable presents the data compilation of material, energy, and process flow, as well as their associated costs, which will be part of the LCI; and the description of the followed steps to create a data base which would be publicly accessible via the VAPO webpage.

2.1. Sources used for the data collection

A template, prepared by Fraunhofer, was distributed to the VIPERLAB consortium on 18 January 2023. It took between four and ten months to receive feedback and answer queries related to the required data before receiving all the contributions. Figure 2 presents the original template that was distributed. The data collection was made possible thanks to the support of some of our VIPERLAB's partners, including CEA, CENER, CSEM, FRAUNHOFER, HZB, IMEC, SU and UNITOV, who provided their own processing data for perovskite single junction and tandem cells. Additionally, data from the bibliography was included to complete the information.

Once all the contributions were obtained, three months were needed to compile all the information in one file and unify all the data into the same units. When necessary, new data fields were incorporated into the file.

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CONFIDENTIAL			Short name
Process steps			Process name
Materials	Main process materials		
	Total Layer Thickness	nm	
	Comment		
Equipment	Type		
	Manufacturer		
	Tool/Platform		
	Amount of Processing Units	#	
	Tray configuration		
	Wafer per Tray	#	
Wafer format	Format		M10
	Area	cm²	330.69
	Efficiency	%	24.0%
	Power	Wp	7.94
Throughput (TP)	Cycle time	s	
	TP capacity	wph	0
		MWp/a	0.0
	Equipment Up-Time	%	100.0%
	Scheduled Down Time	%	
	Unscheduled Down Time	%	
	Gross TP	wph	0
		MWp/a	0.0
	Process Yield	%	
	Net TP	wph	0
		MWp/a	0
CAPEX			
	Process Equipment	Mn EUR	
	Handling/Automation	Mn EUR	
	Metrology Equipment	Mn EUR	
	Total	Mn EUR	0.00
Floor Space			
	Equipment length	m	
	Equipment width	m	
	Handling/Automation	m²	
	Metrology Equipment	m²	
	Total	m²	0.0
Personnel			
	Operation	FTE	
	Technician	FTE	
	Maintenance	h/a	
	Comment		
Maintenance Costs			
	Share of CAPEX p.a.	%	
	Total	k€/a	0
Utilities & Gases (avg. consumption)			
	Electricity	kWh/h	
	Cooling via PCW	kWh/h	
	GEX	m³/h	
	PEX	m³/h	
	Argon	m³/h	
	N2	m³/h	-
	-	m³/h	-
	-	m³/h	-
	-	m³/h	-
Process material consumption/price			
	Production operations time	h/a	8,400
Material 1	Type/Name		
	Consumption		
	Price		
Material 2	Target Type		
	Comment (Target type/composition)		
	Target Price	€/Target	
	Target Consumption	Targets/a	
	Total Material Mass per Target	kg/Target	
	Target utilization	%	
	Usable Material Mass per Target	kg/Target	
	Material Utilization (depos. on substrate)	%	
	Deposited material "on substrate"	mg/Wafer	#¡DIV/0!
	Lost material on tray/walls	mg/Wafer	#¡DIV/0!
	Material consumption per Wafer	mg/Wafer	#¡DIV/0!
Material 3	Type/Name		
	Consumption		
	Price		

Wafer format	M2	M6	M10	G12	G12+
Area (cm²)	244.32	274.15	330.69	440.96	469.46

Figure 2. Template distributed among the consortium.

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2.2. Data unification

The units employed will depend on the source from which the data was obtained. To illustrate, the costs could be expressed in euros, dollars, pounds, etc, which is why it was necessary to unify all data in the same units.

In this way, all the cost values will be represented in euros, using as conversion values those described in the following Table 1.

Table 1. Currency conversion values used to unify collected cost data.

Date of currency conversion	Currency	Symbol	Equivalence in euros
04/01/2024	American dollar (USD)	$	1 $ → 0.91 €
04/01/2024	British pound sterling (GBP)	£	1 £→ 1.16 €

The metric unit of mass for the original data could be given in kilograms (kg), grams (g), or milligrams (mg), while volumes could be in litre (L), millilitres (ml) or microliter (µl). Since most materials are used in very small quantities, the mass and volume units were unified to grams or millilitre, instead of using the international system and give the values in kilograms and litre.

The material consumption data was also given in a variety of units such as mass or volume per batch, substrate, unit, wafer, module, or year, therefore, when the area of the wafer, substrate, module, etc was given the consumption was unified in mass or volume per square meter (g/m^2 or ml/m^2).

3. Database design

This section details the generic steps followed to design the database, from the definition of requirements to implementing security measures and optimizing performance:

1. Determine the purpose and requirements of the database.
2. Choose a database management system.
3. Design the database schema.
4. Create the database.
5. Identify the entities and create the tables.
6. Define the relationships between the entities.
7. Implementation of security measures.
8. Performance optimization.
9. Test the database design.
10. Create a backup and recovery plan.

<u>Determine the purpose and requirements of the database.</u>

The first step is to identify and analyse the project requirements to determine what data will need to be stored, how they will be structured and what functionalities the database should provide. The main purpose of this database is to facilitate the search of information from the LCI, for which data

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compilation and unification was conducted in an Excel sheet, and the requested fields, are those presented in the Table 2.

Table 2. Requested fields for data collection within the VIPERLAB project.

Source		
Layer		
Equipment		
Process steps		
Layer Composition	**Main material (Full name)**	
Materials	Main process materials (Abbreviation)	
	Total Layer Thickness	nm
	Comment	
Year of data collection		
Equipment	Type	
	Manufacturer	
	Tool/Platform	
	Amount of Processing Units	#
	Tray configuration	
	Wafer per Tray	#
Process 1		
	Energy Consumption	kWh
	Time	s
Process 2		
	Energy Consumption	kWh
	Time	s
Wafer format	Format	
	Area	cm^2
	Efficiency	%
	Power	Wp
Throughput (TP)	Cycle time	s
	Cycle time	m^2/h
	Cycle time	wafer/h
	TP capacity	wph
		MWp/a
	Equipment Up-Time	%
	Scheduled Down Time	%
	Unscheduled Down Time	%
	Gross TP	wph
		MWp/a
	Process Yield	%
	Net TP	wph
		MWp/a
CAPEX		
	Process Equipment	Mn EUR
		$M
	Facility cost	% of tool cost
	Spare Parts	% CAPEX/year

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	Handling/Automation	Mn EUR
	Metrology Equipment	Mn EUR
	Total	Mn EUR
Floor Space		
	Equipment length	m
	Equipment width	m
	Handling/Automation	m^2
	Metrology Equipment	m^2
	Total	m^2
Personnel		
	Operation	FTE
	Technician	FTE
	Maintenance	h/a
	Comment	
Maintenance Costs		
	Share of CAPEX p.a.	%
	Total	k€/a
Utilities & Gases (avg. consumption)		
	Electricity	kWh/h
		kWh/m^2
		kW
	Cooling via PCW (Process Cooling Water)	kWh/h
		m^3/h
	GEX (General Exhaust)	m^3/h
	PEX (Process Exhaust going to treatment)	m^3/h
	CDA_CompressedDryAir	m^3/h
	Argon	m^3/h
	Argon-5.0	m^3/h
	N_2-6.0	m^3/h
	DI water	l/h
Process material consumption/price		
	Total	€/m^2
		€/g or ml
	Production operations time	h/a
Material 1	Type	
	Name	
	Consumption	g/m^2
		ml/m^2
		Kg/a
	Coment Consuption	
	Waste of Material	%
	Price	€/m^2
		€/g
		€/ml
	Comment (Target type/composition)	
	Target Price	€/Target

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	Target Consumption	Targets/a
	Total Material Mass per Target	kg/Target
	Target utilization	%
	Usable Material Mass per Target	kg/Target
	Material Utilization (depos. on substrate)	%
Material 2	Type	
	Name	
	Consumption	g/m^2
		ml/m^2
		Kg/a
	Coment Consuption	
	Waste of Material	%
	Price	€/m^2
		€/g
		€/ml
	Comment (Target type/composition)	
	Target Price	€/Target

Choose a database management system.

MySQL was chosen as the database management system because it is widely used, it is open source, and it offers a good balance between performance and features.

Design the database schema.

Once the requirements have been clearly defined, the database schema should be designed using appropriate database design tools. This will involve defining the tables, fields, relationships, and constraints necessary to represent data effectively.

Create the database.

The next step is to create the database in MySQL. This is done by running an SQL command including the desired database name to create it.

Identify the entities and create the tables.

Once the database has been created, the subsequent task is to proceed with the identification of the entities and the creation of the tables in accordance with the previously designed scheme. Therefore, the existing data (Table 2) must be analysed to identify possible entities and separate them into the necessary tables.

Define the relationships between the entities.

Should the database contain related tables, it is then essential to create the relationships between the different tables in accordance with the project requirements. As an example, in Figure 3 the entity relationship diagram is presented. The principal entities identified include layer, material, process, and equipment. Attempting to determine their interrelationships proved to be a complex undertaking. The information collected in the Excel document is of great variety, very specific and complex to interpret if one is not familiar with the subject. Combined with the way the information has been

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organised in the Excel document, this has made it difficult for the IT team to separate the data collected into entities and given the multiplicity of existing correlations, to find the connection or relationship between them to determine the relationship between the defined entities.

One solution could be to implement a data insertion system with a well-defined data model to avoid the complex process of adapting the original dataset (excel).

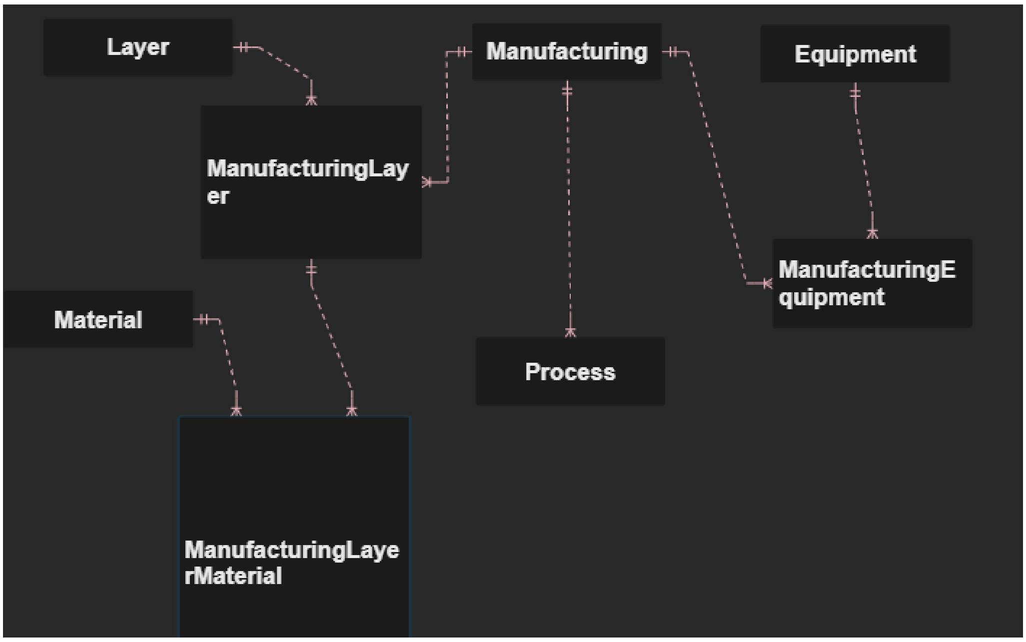

Figure 3. Entity relationship diagram.

<u>Implementation of security measures</u>.

To safeguard the integrity of the database, it is necessary to create users (admin) and assign them specific permissions. Only this *admin* users will have permissions to edit the database and they will belong to CENER's IT department.

The database will be publicly displayed on VAPO's web platform, where all users who visit it will have access to the database. These end users will only be able to consult it and will not have permission to edit it.

<u>Performance optimization</u>.

To enhance performance, indexes are created on columns that are frequently utilized in SELECT queries. Additionally, techniques such as data normalization are employed with the objective of reducing redundancy and improving storage efficiency.

<u>Test the database design</u>.

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Extensive testing is conducted to ascertain the functionality of the database and its compliance with the project requirements. This encompasses data insertion, update, and deletion testing, as well as performance testing.

Create a backup and recovery plan.

A contingency plan must be devised to ensure the periodic backup of the database, thereby guaranteeing the continued availability of data in the event of system failure or disasters.

Once the database has been constructed, the next stage is to consider how it will appear to the end-user. Figure 4 shows the sketch of what the database will look like. The objective was to create an accessible and intuitive user experience. This was achieved by simplifying the interface to facilitate navigation and further searches.

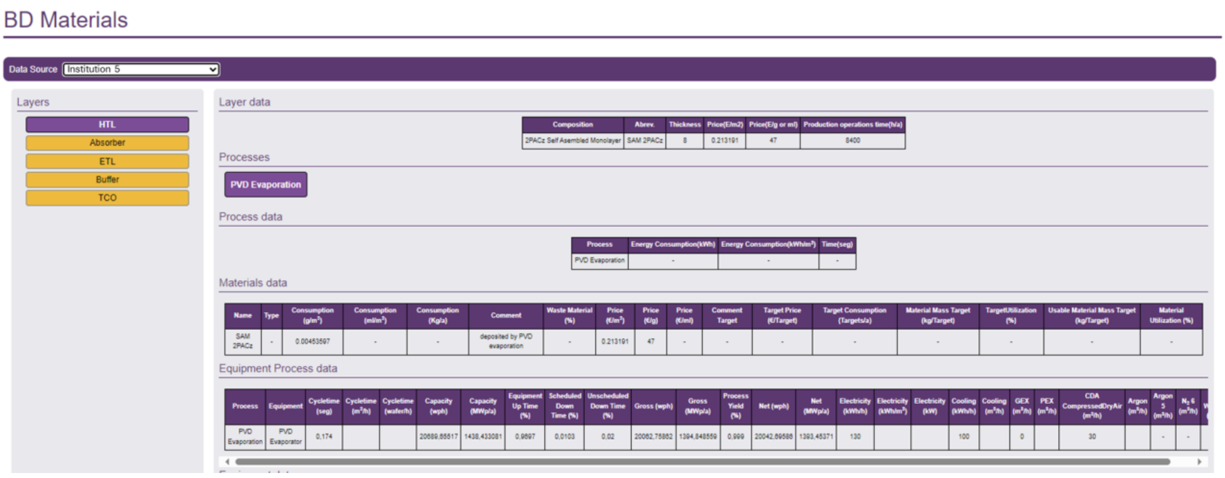

Figure 4. Sketch of the database appearance to end-users.

The database will facilitate more efficient navigation of the collected data, thereby enhancing accessibility and usability of this LCI. One of the objectives is to facilitate a rapid and straightforward search to retrieve information by allowing users to search using previously defined filters.

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4. SUMMARY AND NEXT STEPS

The deliverable report D10.2 within the VIPERLAB project addresses the second task, related to the provision of data on cost, material consumption and processing equipment (parameters such as CAPEX, throughput, yield, etc.) for each material required for carrying out an economic and environmental assessment. With assistance from the VIPERLAB members CEA, CENER, CSEM, FRAUNHOFER, HZB, IMEC, SU and UNITOV, the compilation of data was carried out during the last year followed by the unification of all the data that was obtained. The main effort was to unify the data into the same measurement units, which in some cases has involved directly requesting, from the sources of origin, further information and help in interpreting the data. As a result, all the information has been put together in a single Excel spreadsheet that can be shared upon request among EU and VIPERLAB partners, but it is not as straightforward to extract the information. Therefore, a database is designed, to simplify the search for data. The following steps were to extract from this information the entities and their relationship to design the database, a task that proved challenging given the different nature of the data.

The third task is to provide the environmental Life Cycle Assessment social and economic Levelized Cost of Electricity impact assessment of the selected device architectures with the chosen materials. The results of such an assessment will contribute significantly to VIPERLAB's overall goal of establishing EU-based perovskite PV production with the lowest cost and lowest carbon footprint.

5. PUBLICATION BIBLIOGRAPHY

[1] European Commission. European platform on LCA https://eplca.jrc.ec.europa.eu/lifecycleassessment.html (accessed Apr 3, 2024).

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