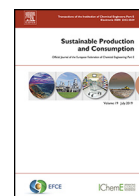




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Research article

A set of principles for applying Circular Economy to the PV industry: Modeling a closed-loop material cycle system for crystalline photovoltaic panels

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ABSTRACT

The growing popularity of crystalline silicon photovoltaic (C-Si PV) panels will generate a massive amount of waste when they reach their end-of-life (EoL) phase. For sustainable energy technology, we must implement an effective solar photovoltaic (PV) material recovery system. In this paper, the authors assess a Circular Economy (CE) system based on Cradle-to-Cradle (C2C) philosophy as an alternative to tackle the daunting challenge of this waste and explore its impacts in the form of a Closed-Loop Material Cycle (CLMC). First, we discuss the novel concept of circular time, and material separation of C-Si PV materials is discussed by theoretically introducing a novel framework. Then, we recreate a numerical simulation experiment to evaluate the performance of the proposed theoretical model of a CLMC to assess the flow of silicon used in C-Si PV, aiding in future planning and logistics for a CE in the PV industry. The preliminary results obtained in the simulation show that it is not possible to close the material flow without introducing new raw material into the system, unless the operational lifespan of the PV panels is reduced.

This research seeks to fill a gap in CE theoretical literature by introducing a new framework and identifying some of the challenges and limits of implementing a CE system in the form of a CLMC system based on C2C principles (C2C-CLMC).

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1. Introduction

The world is undergoing a massive transition from a predominantly carbon-based energy system dependent on fossil fuels towards a low-carbon energy system dominated by renewable energy (RE) technologies. Solar photovoltaic (PV) panels are one of the most widely used RE technologies, with a global record of 98 GW of installed capacity and connected to the grid in 2019 (IRENA, 2020), representing approximately 23 percent of all globally installed RE power capacity in 2019 (IRENA, 2020). The global cumulative capacity installed until 2019 was about 635 GW (ISE, 2020) and it is projected to increase to approximately 1337 GW by 2025 (IEA, 2020). In this context, Silicon (Si) wafer PV technology represents about 95 percent of the total PV technology production in 2019 (ISE, 2020). Renewable energy and solar PV tech-

nology in particular have been growing exponentially, mostly because of climate change and new policies adopted by many countries to cut carbon emissions after the Paris Climate Accords in 2015. High demand on materials needed to manufacture renewable energy technologies is already compromised by dramatic rates of PV panels and other RE technologies production, constraining the possibility of achieving the clean energy system ambitioned by 2050 (Moreau et al., 2019).

The increasing demand for PV technology described above, along with panels that have an average operational life of 25 to 30-years (Deng et al., 2019), will result in large amounts of waste when panels reach the end-of-life (EoL) phase, around 78 Mt of solar PV waste by 2050 (Chowdhury et al., 2020). Moreover, C-Si PV panels are a highly competitive renewable energy technology that has evolved rapidly in the last decade. They boast a fifteenfold reduction of cost from 2008 to 2019 (Green, 2019) and have increased efficiencies from 5% in 1950 to the record lab efficiency of 26.7% in 2020 (Green et al., 2021). Furthermore, the global energy transition towards renewables comes with an increased demand for mineral production by around 200–900% from the electricity

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Nomenclature

A	Helmholtz free energy
A_i^o	Molar Helmholtz free energy
A_{pi}^o	Molar Gibbs energy
dN_i	Set of moles of i components
δW_b	Boundary work
δW_{rev}	Reversible work
δW_s	Shaft work
N_{mi}	Total number of moles mixture
N_{pi}	Total number of moles pure components
A_m	Total Helmholtz free energy
P	Pressure
μ_{pi}	Chemical potential pure materials
T_c	Circular time
T	Temperature
T_{ind}	Industrial time
T_d	Dwelling time
T_{rr}	Removal and recovery
T_{rs}	Reservoir time
R	Constant gas
W_m	Minimum work separation random mix
$\frac{\partial}{\partial x}$	Space derivative
$\frac{\partial}{\partial t}$	Time derivative
$\bar{\rho}$	Average material density
\bar{u}_i	Average processing velocity at \hat{i}
$\frac{\bar{\rho}_i^{n+1} - \bar{\rho}_i^n}{\Delta t}$	Numerical approximation for $\frac{\partial \bar{\rho}}{\partial t}$
$\frac{\bar{\rho}_i^n \bar{u}_i - \bar{\rho}_{i-1}^n \bar{u}_{i-1}}{\Delta x}$	Numerical approximation for $\bar{u}_i \frac{\partial \bar{\rho}}{\partial x}$
$\tilde{\rho}_2^{n+1}$	Joint point of the system
$\bar{\xi}_n$	Average processing rate of $\bar{\rho}$
$\bar{\rho}_i \bar{u}_i$	Flux of S_i

sector between 2015 to 2050 (Watari et al., 2019), highlighting the importance and the urgency for improving material efficiency and management and moving towards a circular paradigm, otherwise, the energy transition may become unsustainable.

C-Si PV panel technology depends on the availability of valuable metals, including Si. For instance, demand estimations for Si in Europe will grow in a high-PV deployment scenario, from 42,854 t in 2020 to 234,962 t in 2030 (European Commission, 2018). Hence, improving Si's efficient management throughout its EoL may help to ensure supply in the PV industry. Moreover, the Waste Electrical and Electronic Equipment (WEEE) Directive 2012/19/EU has signaled a way in that sense, and has pushed for the development of PV recycling facilities in the EU (EC, 2012).

Researchers have already recognized the importance and need for a comprehensive recycling system (i.e. logistics, recycling, storage, and sustainable waste treatment) for all materials within PV modules (Xu et al., 2018), achieving economic feasibility and reducing environmental impacts (Deng et al., 2019), while promoting a PV closed material cycle may be able to improve resource efficiency and waste reduction (Sica et al., 2018). Moreover, the manufacturing of a crystalline solar cell entails several steps (Woodhouse et al., 2019), where, after a multistage distillation process (Siemens process), the polysilicon is transformed into cylindrical ingots of monocrystalline Si, which are then shaped and sliced into thin wafers (Woodhouse et al., 2019). Hence, the highly-pure and energy-intensive Si used in the PV industry is a valuable material (Deng et al., 2019), and this is why the main focus of our research is about the EoL of the Si confined in a crystalline PV panel.

Contreras-Lisperguer highlighted the importance of transitioning away from recycling, which has become a key stage at the EoL

of the linear paradigm Cradle-to-Grave (C2G). In C2G, the lifetime of PV panels is linear, from the extraction of material used in manufacturing them (cradle) until EoL where they are considered waste (grave), and only a fraction of its raw materials reaches the recycling phase. In up-cycling, which is a concept based on the circular paradigm Cradle-to-Cradle (C2C), all materials are used indefinitely, and at EoL, they can become a primary resource to manufacture another panel (Contreras Lisperguer et al., 2020). More details about C2C and C2G principles are available in Appendix A *Linear versus Circular: Cradle-to-Grave and Cradle-to-Cradle*. Consequently, recycling is not an appropriate solution to solve waste accumulation and the environmental challenges ahead since recycled materials were already considered waste. This option is conceptually flawed from the outset. Furthermore, Non-Renewable-Abiotic-Primary-Resources (NRAPR) are viewed as non-renewable stock (Schulze et al., 2020), which is why it is important to minimize our reliance on these limited resources by recovering them at the EoL. Here, NRAPR has been defined as natural sources (including energy sources), such as minerals, metals, iron ore and crude oil, which are considered stock in the environment that is “depleted through physical extraction of resources (mining and subsequent processing) from the environment into the economy” (Schulze et al., 2020). CE, particularly in the form of a Closed-Loop Material Cycle (CLMC), not only could potentially reduce competition over these resources, but also make better use of them and the key role of redesign and design for recovering and recycling in a sustainable CE system (Velenturf and Purnell, 2021). However, given the complexity of creating and implementing a C2C-CLMC system, together with the impracticability of conducting experiments on the supply chain and logistic systems at the global or regional scales, we must develop a credible scientific framework for system modeling based on thermodynamics and mathematics to stimulate research and recognition in the academic community.

In this article, we introduce a new theoretical framework that stably simulates and forecasts the material flow of Si at a global/hemispheric scale for a C2C-CLMC system. We hope our study leads to a wider use of inductive methods in this transition from a linear to a circular economical system. The article is divided as follows. First, in Section 2 we present a literature review that provides the context for our research. Then, in Section 3, we discuss the methodologies used in this research. In Section 3.1, we introduce the energetic and thermodynamic implications of material separation in a system. In Section 3.2 we propose a new procedure to comprehend material separation for a C2C-product. Afterward, in Section 3.3, we address the challenge of time and space scales interactions by defining a suitable one, and at Section 3.4, we formulate the concept of circular time (T_c) and its various components. A description of *Dwelling time* (T_d) is provided in Appendix B *Dwelling time estimation*. The mathematical part in Section 3.5 is devoted to contemplating the right set of equations that describe a C2C-CLMC system. A detailed description of the conservation of mass equation is provided in Appendix C *Conservation of mass equation and its linearization*, and the stability analysis of our model is provided in Appendix D *Stability analysis of our model*. Then, in Section 3.6, we incorporate a numerical simulation to test our model at hemispheric scale. Finally, preliminary assumptions and boundary conditions are introduced at Section 3.7, while a detailed calculation of T_d for crystalline silicon photovoltaic PV panel is available in Appendix E *Estimating Dwelling time for a crystalline silicon photovoltaic panel*. In Section 4, we present a numerical simulation of the test results. As an alternative to the classic sensitivity analysis a brief note using a *simplified ensemble analysis* on the variations of T_d is available in Section 4.1. Finally, we elaborate on our conclusions and recommendations in Section 5.

2. Literature review

Today's PV industry is consuming Earth's NRAPR, generating massive amounts of waste at the EoL of manufactured PV panels. This waste provokes several broad environmental impacts: eutrophication, mineral depletion, loss of biodiversity, and CO₂ emissions (Contreras Lisperguer et al., 2020). Consequently, sustainable recycling methodologies for C-Si PV panels are essential to move towards a sustainable Circular Economy (CE). Briefly summarized, a C-Si PV panel structure is composed of many electrically connected solar cells with Ag contacts on the front and back, coated with an ethylene vinyl acetate (EVA) layer, which acts as electrical insulation. This electrical insulation provides the solar cell with protection from the environment and increases its lifespan. This structure is heated until is sealed, then it is covered by glass, and the laminated structure is encased in an aluminum frame (Gorjian and Ashish, 2020). This kind of sandwich structure, particularly the use of EVA, poses a major challenge when it comes to recovering and recycling the materials used in the C-Si PV panel manufacture because it can only be undone by using either a thermal or chemical process, and sometimes a combination of both (Farrell et al., 2020). Thus, generation and accumulation of waste coming from PV panels and other RE technologies is set to become a global challenge in the decades to come.

A typical mass composition of 1000 kg of C-Si PV panel material is approximately 70% glass, 18.5% aluminum, 5.1% EVA, 3.65% Silicon, 1.5% Back foil sheet, 0.11% Cooper, 0.053% Silver, 0.035% Led, and 0.018% Tin (Contreras Lisperguer et al., 2020). Recovering and recycling all those materials embedded in a panel may have alternative pathways that can be categorized into physical, thermal, and chemical treatments and/or a combination of those treatments (Chowdhury et al., 2020). Thus, the efficiency of the recycling process at EoL will depend on the effectiveness of the chosen treatment for recycling, and this is especially challenging due to the enclosed nature ("sandwich" structure) of the C-Si PV panel structure (Farrell et al., 2020), nevertheless, a piloting recycling methodology for C-Si PV panels has achieved around 95% of recycling rate for Si (Contreras Lisperguer et al., 2020). However, despite the importance of recycling methodologies at the EoL, especially for a CE system, there is very limited data available (Ardente et al., 2019), nonetheless, these recycling technologies are still in their infancy. Many PV panel recycling facilities are still in their pilot stage and very little is known about their environmental impacts (Contreras Lisperguer et al., 2020).

Physical treatment is a mechanical process that usually consists of crushing and grinding the panel after the aluminum frame, cables, and electric box have been removed (Chowdhury et al., 2020). Hence, the physical treatment is rather limited for the recovery of valuable materials, allowing only the recovery of primarily aluminum and glass (Padoan et al., 2019). Thermal treatments use high temperatures to remove the EVA to access the PV cell (Contreras Lisperguer et al., 2020). This treatment is typically carried out by pyrolysis, but is highly energy-intensive, which makes it a less viable option from an economic and environmentally sustainable point of view (Padoan et al., 2019). A chemical treatment entails another option to remove the EVA and to recover valuable metals. This approach usually requires the use of different organic solvents to remove the EVA (Chowdhury et al., 2020). Nevertheless, most of the recycling pathway treatments for C-Si PV panels are a combination of the physical, thermal, and chemical treatments briefly described above (Padoan et al., 2019). Moreover, it is essential to assess the related environmental impacts of all the different treatments pathways, and the Life Cycle Assessment (LCA) methodology is considered to be an effective tool to assess such impacts generated during the recycling of C-Si PV panels used by researchers and academia (Ardente et al., 2019).

In a recent study (Contreras Lisperguer et al., 2020), we investigated the alternative recycling pathways at EoL and its environmental impacts. Furthermore, we provided a thorough estimation of the environmental impacts and potential alternatives to reduce the environmental impacts of the recycling process. We highlighted the potential benefits of a C2C-CLMC scenario as a way to move towards a CE, however, minimizing impacts coming from current energy-intensive thermal treatments and toxic chemical treatments continues to be a top priority for the enclosed sandwich nature of current silicon PV modules. For instance, in terms of environmental impacts, the recovery of PV materials in a C2C-CLMC scenario results in the reduction of the Climate Change impact factor (kg CO₂ eq) by 74% compared to an Open scenario (Contreras Lisperguer et al., 2020). In any case, it is necessary to consider new design pathways that facilitate disassembly, recovery of materials, and the entire recycling process.

Modeling the material cycles and flows is considered a critical step for resource management and sustainability. Material Flow Analysis (MFA) can be defined as a quantitative exercise based on the principle of mass conservation for studying the flows and stocks of natural resources and materials within a given system, and can be applied at various space and time scales (Zhang, 2019), where flows are usually given by kilogram per year (kg/yr) (Kapoor et al., 2020). MFA can be considered a component of the LCA tool, and provides a snapshot in time of the environmental impact of the different processes involve by weighing each material. The results provides a C2G accounting of the direct and indirect material flows involved in the production of a product or delivery of a service (Zhang, 2019), and can provide useful information for policy makers.

Studies using LCA models and MFA assessed the efficiency related to the recycling process for c-Si PV waste. These results illustrate material flows for the PV recycling process based on the average practices in Western European WEEE recycling plants whose overall recycling rate is around 24%, which is well below the current minimum target of 80% (in mass) of reuse and recycling set by the WEEE Directive (Ardente et al., 2019). One research project even achieved an estimated recycling rate of 83% using a novel recycling process for c-Si PV panels (Ardente et al., 2019).

The importance of increasing recycling performance for C-Si PV panels at the commercial level is paramount to successfully implementing a C2C-CLMC in the PV industry. This becomes even more important when considering that recent research indicates, for example, that the highest amount of PV waste in Australia will come from crystalline silicon-based PV panels, reaching around 80% by 2047 (Mahmoudi et al., 2019), while for the OECD countries it is estimated to reach about 29 million tons of PV waste by 2058 (Mahmoudi et al., 2021).

The potential today to upcycle C-Si PV in a C2C-CLMC system is still limited because PV panels have not been designed to be recovered and reused at EoL (Contreras-Lisperguer et al., 2017), however, silicon-based PV panels are manufactured mostly with highly pure Si (Deng et al., 2019), and valuable materials (e.g. copper, aluminum, silver, etc.) (Ardente et al., 2019), therefore, the potential reuse of those materials can be technically feasible, however, there is very limited research conducted on the resource efficiency in the recycling of such valuable metals (Ardente et al., 2019). Furthermore, in a C2C-CLMC system such as a CE, the key is to weigh the physical availability of all materials, particularly for recycling, recovery, and reuse at EoL. That way, modeling material cycles and flows become important tools for resource management and sustainability (Balanay and Halog, 2018), achieving resource efficiency, and reducing competition on access to raw materials and their supply (Penaherrera and Pehlken, 2020). However, some indicators used in methodologies such as material flow analysis and life cy-

cle assessment are inefficient in consider the temporal variations of material stocks (Penaherrera and Pehlken, 2020).

On the other hand, a growing body of literature examines the use of dynamics models based on partial differential equations (PDE). These models have mainly been used to describe material flow in manufacturing facilities (Glatt et al., 2018), supply chains models (Yuan et al., 2020), game theory approach (Chen et al., 2021), and optimal control of supply chains models (Rarità et al., 2021), while other studies provide some generic considerations for modeling and simulation for an end-to-end supply chain system (Chilmon and Tipi, 2020) or the theoretical stability of the conservation laws based on PDE in numerical simulations (Chiarello et al., 2019). Previous work in material flow using dynamics models based on PDE indicated above has mostly focused on modeling material flow at the theoretical level in small facilities at local space-scales (i.e. factories, conveyor belts, manufacturing processes) and at local time-scales (e.g. seconds, hours and days of some manufacturing process). Furthermore, the latest research available on the study of closed-loop systems has mostly focused on the use of mathematical-statistics, such as multi-objective evolutionary algorithm (Cheraghalipour et al., 2018), optimization models (Accorsi et al., 2020), network models (Fu et al., 2021), and game theory (Shekarian and Flapper, 2021).

Despite the interest, no one to the best of our knowledge has studied the topic of dynamics simulations using PDE of material flow for products with a long operational life-cycle (i.e. 25–30 years) on a large spatial-scale (i.e. thousand kilometers on a hemispheric-scale), like commercial PV panels used in large solar power plants. We have yet to consider a holistic analysis of the thermodynamic implications in material separations under the C2C framework.

Incapability to perform experiments with real-time material flow in the real world warrants a need to develop a deeper understanding of this issue. In this scenario, material flow simulation methods are essential for the understanding and implementation of a complex C2C-CLMC system at a global scale. Further, such simulations are also needed for strategic decision-making purposes, since material flow patterns provide vital information for logistics, planning, and material control.

Modeling systems can help to improve the knowledge, without disturbing the PV industry, about the limitations and implications of applying new paradigms such as CE in our industrial-economic systems before implementing them (e.g. measurements, storage, balance of the material, time, and space scales, etc.). A proper transition from a linear to a circular economical system requires developing a proper theoretical model based on mathematics and thermodynamics (Contreras-Lisperguer et al., 2017).

The first step towards the implementation of a C2C-CLMC system involves laying out the necessary theoretical framework to do so. A sound C2C-CLMC system design first requires a robust theory based on mathematic and thermodynamic principles, but little is known about the implications of a C2C-CLMC system at the global/hemispheric level.

3. Methods

It is expected that if well-designed under C2C principles, a C-Si PV panel at EoL will contain high-quality primary resources. The C2C approach promotes a circular industrial symbiosis based on the central equation “waste = food”, whereby all materials are used indefinitely (Braungart et al., 2007).

A CLMC system based on the C2C philosophy (C2C-CLMC) promises to reduce or even eliminate the very concept of waste. Toxic residues would also be completely replaced by non-toxic alternatives and/or effectively encapsulated to prevent any interaction with the environment if the manufacturing sector can im-

plement proper design and values based on a consistent theory. Despite the clearness and optimism behind that assertion, there are serious obstacles other than just planning the implementation of a Closed-Loop supply chain for PV that includes recycling. A fundamental question still needs to be answered. Do we actually know the implications of the laws governing the material flow in a C2C-CLMC system principles? This question can be answered only by deducing consequences from hypothesis and subjecting them to experimental verification. Since it is practically impossible to experiment with the material flow in a supply chain at a global/hemispheric scale, and since an adequate technique is lacking for simulation experiments at a global/hemispheric scale, a theory describing what the material flow will do under a given set of circumstances can be tested only by integration of the appropriate set of equations in a numerical simulation. In the following section, we introduce a technique to dynamically model the material flow of Si based on a time-space scale and thermodynamic analysis that can be applied to any material at a global/hemispheric scale.

3.1. Circular economy system energetics and thermodynamic implications

Before introducing the mathematical model, we must have theoretical evidence of the restrictions on a CE in the form of a C2C-CLMC system. Since a C2C-CLMC is a thermodynamic closed system, our main interest focuses on the conservation of mass, rather than the transformation and exchange of energy within the system and its surroundings. Energetics aspects of a C2C-CLMC system are very important and an exhaustive analysis is outside the scope of this study. However, in this subject it is important to remark that the increasingly accessible, low-entropy energy sources (i.e. solar) can effectively satisfy most of the C2C-CLMC's future energy needs. Furthermore, it has been already proven that a CLMC system is not limited neither by its energy needs nor by the second law of thermodynamics (Ayres, 1999). Moreover, we suggest that the work needed at EoL may be significantly less with C2C-products compared with non-C2C-products that require special treatment, consume of large amounts of energy and generate toxic residues.

Ideally, a C2C product must be designed with the upcycling phase in mind for all materials used in the product. Putting this system into actual practice requires greatly improving the effectiveness of material selection and material recovery and reutilization¹. Therefore, a C2C product should comply with some requirements that facilitate future upcycling:

- Materials should be carefully selected during the design phase with EoL in consideration by combining the strength of both C2C certification and LCA tool (Contreras-Lisperguer et al., 2017). Furthermore, C2C practitioners should consider the value of LCA methodology, addressing the trade-offs between resource conservation and energy use (Bjørn and Hauschild, 2013).
- All toxic materials must be replaced with non-toxic alternatives. They could also be effectively encapsulated (less ideal situation).
- The product's disassembly phase must be as efficient and effective as possible.

The requirements explained above are not telling us much about the physical restrictions that a C2C-product may face during the disassembly phase. To explore these restrictions, the work required to separate the materials contained in a C2C-product at

¹ Out of the five C2C-principles, this article focuses primarily on upcycling (or reutilization) materials.

EoL merits further analysis. In the following section we analyze the thermodynamic implications of material separation in a C2C-product.

3.2. Separating materials of a Cradle-to-Cradle versus a non-Cradle-to-Cradle products

From a thermodynamic point of view, a PV panel designed under the C2C principles can be regarded as a non-random mixture of different pure components. If these building blocks are systematically distributed and ideally sustain the same volume, we would significantly reduce any increase in entropy of the component mix. Because of this, we propose the following theory:

Conjecture. The work necessary to separate the components in a fully designed C2C PV panel can be considered minor compared to the amount of work needed for a PV panel designed without a C2C concept. We verify our initial conjecture below.

Proof. Consider two pure components, in this case two ideal gases. We assume that each of these components is restricted to an equivalent volume that is regular. If we then consider the reversible equation for the total isothermal work for a non-reactive system, it can be written as follows for two components,

$$\delta W_{rev} = \frac{\partial A}{\partial P} dP + \sum \mu_{pi} dN_i + \sum A_i^o dN_i \quad (1)$$

where A is Helmholtz free energy, P is pressure, μ_{pi} is the chemical potential of the pure materials, A_i^o is molar Helmholtz free energy, and dN_i is the differential number for the complete set of moles of i components. In addition, we consider that all mole numbers remain fixed. In this system $\delta W_{rev} = \delta W_b + \delta W_s$, where δW_b is the boundary work and δW_s is the shaft work, however, since the capacity-unit does not change in the separation process, we can fairly assume the boundary works to be zero, therefore, the total work is only the shaft work. Hence, we can rewrite equation (1) as

$$\delta W_s = \frac{\partial A}{\partial P} dP + \sum \mu_{pi} dN_i + \sum A_i^o dN_i \quad (2)$$

Since we know that for a pure component, the chemical potential (μ_{pi}) is the molar Gibbs energy (A_{pi}^o) (Burghardt and Harbach, 1993), then we can re-write equation (2) as

$$\delta W_s = \frac{\partial A}{\partial P} dP + \left[\sum A_{pi}^o + \sum A_i^o \right] dN_i \quad (3)$$

therefore, by using the ideal gases equation and applying the chain rule on $\frac{\partial A}{\partial P} dP$, then, the first term of equation (3) becomes

$$\frac{\partial A}{\partial P} dP = \sum RT dN_i = 0 \quad (4)$$

Consequently, since (4) is equal zero, then, equation (3) becomes

$$\delta W_s = \left[\sum A_{pi}^o + \sum A_i^o \right] dN_i \quad (5)$$

If the components are extracted throughout the separation, then equation (5) can be directly integrated to yield

$$W_s = \sum_i \left[A_{pi}^o(T, V, N_{pi}) - A_i^o(T, V, N_{mi}) \right] N_i \quad (6)$$

Where N_{pi} is total number of moles of the pure components, N_{mi} is total number of moles in the mixture, and N_i represents the total number of moles of component i in the vessel at the start of the separation process. Here, using the Gibbs-Duhem equation (Astarita, 1993) for the mixture, then, we can define

$$A_m = \sum_i N_i A_i^o \quad (7)$$

Where A_m is the total Helmholtz free energy of the original mixture. Introducing (7) on equation (6), we can rewrite it as

$$W_s = \sum_i N_i A_{pi}^o(T, V, N_i) - A_m(T, V, N_{mi}) \quad (8)$$

If we define the intensive property of A_{pi}^o as $a_{pi} = \frac{A_{pi}^o}{N}$, where N is the total of moles in the mixture, by introducing a_{pi} in equation (8), we can rewrite (8) as

$$W_s = \sum_i a_{pi}(T, V, N_i) - A_m(T, V, N_{mi}) \quad (9)$$

Applying the defined intensive property, we obtain the solution to (9) by substituting A_m as the summation of the corresponding a_{pi} of the pure constituents (Guggenheim, 1986)

$$A_m(T, V, N_{mi}) = \sum_i a_{pi}(T, V, N_i) \quad (10)$$

and hence

$$W_s = 0 \quad (11)$$

The method we describe above offers a formal solution (11) with compelling support to establish that there is a possibility to reduce the energy needed to separate the materials embedded in a C2C-PV panel or any other C2C product. Nevertheless, the amount of work needed to separate the materials is smaller compared to the amount of work needed to separate the materials from a non-C2C-product due to the random intermixture of materials, where the minimum work needed is given by $W_m = RT[\ln \frac{1}{x}]$ (Gutowski, 2008), where R is the gas constant and T is temperature.

Our solution, however, unveils a fundamental limitation for a C2C-CLMC system. In order to achieve a minimal work during the material separation phase, the materials used in the product must be highly pure, something that coincidentally is not a burden for C-Si PV panels. Results highlight that there is a lack of forethought in the design of C-Si PV panels and material recuperation at the EoL. Only a few of their components can be recovered in disassembly (Choi and Fthenakis, 2014). The PV industry is currently trying to recover materials for reuse by applying a combination of physical, thermochemical or combined treatments (Chowdhury et al., 2020). They are not solving the problem but rather increasing the inefficiency and toxicity of current recycling practices in the PV industry. We must urgently rethink product design if we want to take advantage of the C2C philosophy and the benefits it provides.

We initially propose that in order to make C-Si PV panel technology more circular and sustainable, the industry would have to comply with three elementary principles:

- 1 Apply C2C philosophy during the design phase for crystalline PV panels following the C2C standards for products (C2C Products Innovation Institute 2016) by substituting poor recyclable materials (e.g. EVA layer), replacing and/or encapsulating toxic materials (Braungart et al. 2007), and applied the sustainable LCA tools to reduce potential environmental impacts during the entire life cycle, particularly at the EoL (Latunussa et al. 2016b);
- 2 Based on our thermodynamic result, the C-Si PV panels should be manufactured with the highest purity of materials today, however, low purity materials will be necessarily neglected. Therefore, closing the material flow per se does not guarantee environmental sustainability;
- 3 Power C-Si PV panel upcycling plants with low-entropy sources, i.e. solar energy.

By following these guidelines, we would reduce the environmental impacts from the overall C-Si PV panels lifecycle, facilitate

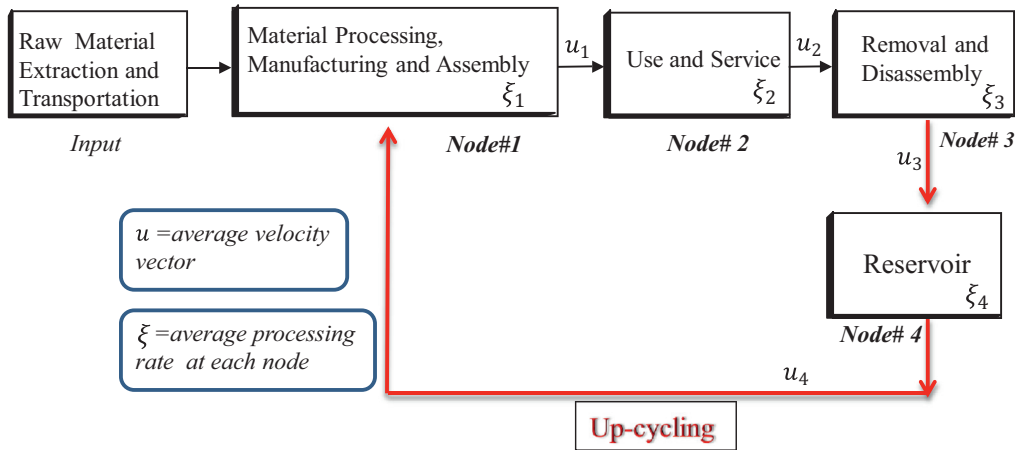


Fig. 1. A simplified closed-loop material cycle system (Adapted from Contreras-Lisperguer et al. 2017)

the disassembly phase, and support the development of new business models, but we must also pay attention to the infrastructural challenge of moving from recycling to upcycling.

Along with the task to reduce the amount of work needed to separate the materials of a product at the EoL, the time-space scales of these processes involved in the lifecycle of a PV panel are crucial to understand the circular flow of material in a C2C-CLMC system.

3.3. Space and time scale

Since there are many processes involved in the lifecycle of a product that differ in space-size and duration (e.g. primary resources extraction, manufacturing, transportation, EoL, etc.), therefore, understanding the horizontal dimensions (spatial scale) and length of time of material flow (time scale) is important. In this article, we used the same space-time scale as described by Contreras-Lisperguer (Contreras-Lisperguer et al., 2017). We pay special attention to the circularity embedded within time-scales related to a C2C-CLMC system. In the following section we define the time-scale as a function of its circularity, which simplifies understanding a quantitative study of a C2C-CLMC system.

3.4. Circular time

A C2C-CLMC system essentially denotes the flow of materials in circles. Therefore, we define circular time (T_c) to denote the particular temporal dimension of material flow in a C2C-CLMC system. For the purpose of this analysis, T_c consists of two main components: industrial time and dwelling time.

- Industrial time (T_{ind}) measures the length of time from the extraction of NRAPR, material transformation and processing, to the end of manufacturing and sale to the consumer. For the most part, T_{ind} should be known for established industrial sectors (i.e. PV industry).
- Dwelling time (T_d) describes the time the finished product stays with the consumer before being returned to the technical cycle as a primary resource. In the case of C-Si PV panels, T_d represents the operational lifespan of the panel. A mathematical description of T_d is provided in the Appendix B. Dwelling time estimation.

In addition, we need to consider the time needed for removal and recovery (T_{rr}) and the time materials will spend at the reservoir (T_{rs}) before returning to the industrial sector for reutilization or “upcycling”. For details see Fig. 1.

Consequently, the circular time for the complete cycle, represented by T_c , can be defined as:

$$T_c = T_{ind} + T_d + T_{rr} + T_{rs} \tag{12}$$

This spans the total duration from initial resource extraction to the beginning of upcycling, which marks the start of a new cycle.

In the following section, we present the treatment of the right set of equations.

3.5. Numerical scheme solution for a Closed-Loop Material Cycle system based on Cradle-to-Cradle principles

In a C2C-CLMC system, materials should flow in a manner that ultimately forms a closed loop. The physical constraint on material flow can be expressed in terms of the equation for conservation of mass.

Due to the complexity of a C2C-CLMC system, a purely analytical solution to the conservation of mass equation (13) is not attainable, therefore, a computational simulation based on numerical methods is necessary to find a solution to our model. A description of equation used in this section is provided in the supporting information section C. Conservation of mass equation and its linearization.

For numerical simplicity and due to limited processing power, our numerical scheme will be defined as a one-dimensional (1-D) system, and it can be written as

$$\frac{\partial \tilde{\rho}}{\partial t} + \tilde{u}_i \frac{\partial \tilde{\rho}}{\partial x} = 0 \tag{13}$$

Where $\tilde{\rho}$ represents the average material density in terms of ρ per units of length and \tilde{u}_i defines the average one-dimensional processing velocity at every stage of the life-cycle of a product.

In order to numerically solve equation (13), we have chosen an explicit donor-cell finite-difference approximation technique to derive its discrete representation and a backward scheme to numerically solve it for the space derivative $\frac{\partial}{\partial x}$, because this is regarded as more stable for $\tilde{u} > 0$ (Durrant, 2010). The stability analysis of our numerical scheme can be found in the supporting information section D. Stability analysis of our model.

The discretization scheme for equation (13) can be written in the following form:

$$\frac{\tilde{\rho}_i^{n+1} - \tilde{\rho}_i^n}{\Delta t} + \frac{\tilde{\rho}_i^n \tilde{u}_i - \tilde{\rho}_{i-1}^n \tilde{u}_{i-1}}{\Delta x} = 0 \tag{14}$$

$$\mathcal{F}(x, t) = \tilde{\rho}(x, t) \tilde{u}(x, t) = \tilde{\rho} \tilde{u}_i(x, t) = \tilde{\rho} \tilde{u}(x, t) \tag{15}$$

If we define

By introducing (14) in equation (15), we may rewrite the scheme as

$$\frac{\tilde{\rho}_i^{n+1} - \tilde{\rho}_i^n}{\Delta t} + \frac{\mathcal{F}_i^n - \mathcal{F}_{i-1}^n}{\Delta x} = 0 \tag{16}$$

In equation (16) x and t are discretized with uniform values of Δx and Δt , respectively. For brevity, we use the notation e.g. $\tilde{\rho}_i^n = \tilde{\rho}(i\Delta x, n\Delta t)$ with $i, n \in \{0, 1, 2, \dots\}$

If we say $\beta = \frac{\Delta t}{\Delta x}$, then we can rewrite (16) as

$$\tilde{\rho}_i^{n+1} = \tilde{\rho}_i^n - \beta(\mathcal{F}_i^n - \mathcal{F}_{i-1}^n) \tag{17}$$

The resulting numerical scheme (17) serves to model the flow of an imaginary and arbitrary volume of Si in a C2C-CLMC system. However, in order to complete our numerical scheme, we must close the material flow. The numerical solution proposed to close the loop for our C2C-CLMC model has been solved by introducing a joint point. The joint point represents in the numerical scheme the transportation process of the recovered materials from the reservoir to the industrial facility for reuse. Therefore, the strategy here is to connect the EoL phase with the recovered material processing facility in terms of material flow. The joint point we have defined has the following form

$$\tilde{\rho}_2^{n+1} = \tilde{\rho}_2^n - \beta[\tilde{\rho}_2^n \tilde{u}_2 - (\tilde{\rho}_1^n \tilde{u}_1 + \tilde{\rho}_{end}^n \tilde{u}_{end})] \tag{18}$$

Equations (17) and (18) are the numerical solution of the governing equation of our C2C-CLMC system. Its solution may be found by numerically solving for $\frac{\partial \tilde{\rho}}{\partial t}$ and extrapolating the motion forward in time of the material flow, but the initial and boundary conditions must first be established. In the following section we introduce the initial and a numerical experiment that will help to test the reliability and stability of our model at a global/hemispheric performance scale.

3.6. Numerical simulation tests

In order to assess the stability and convergency of our proposed numerical method described in the previous section, we made assumptions to test our model in the form of a numerical experiment. However, it would be very demanding to simulate and render the material flow and processing facilities of all C-Si PV panels produced in the world using high-resolution three-dimensional structural data, and appropriate machine representations. This is due to the very high computing power that will require such modeling. Therefore, in this numerical test, we do not attempt to model the global PV industry because that would be beyond the scope of this research. The goal of this preliminary exercise is to shed some initial light on the challenges that may exist in the supply chain when trying to implement a Circular Economy in the PV industry. We hope that this model can be applied in future research to contribute to the understanding of a Circular Economy in the photovoltaic industry.

The boundary conditions and initial assumptions imposed in this numerical test are made in order to facilitate the processing of numerical discretization solution and numerical calculations. The simplified assumptions and boundary conditions will help us confirm if the proposed model is stable, if the system is able to close the material cycle without inputting new raw material from an external source, and to assess how long it would take to do so. In this simplified numerical test, we have simulated a case, performed in one-dimension (1D) for a C2C-CLMC system, in which PV material (Si) is added into a closed system, for any given single year, simulating its entire life-cycle of material flow for Si , from the input of material extracted from a mining process into the manufacturing facility, PV manufacturing, use, decommissioning, recovering, reservoir, and reuse as a raw material in the manufacturing sector (upcycling) in a C2C-CLMC system. Here, PV panels adhere to

the thermodynamic implications of material separation in a C2C-product introduced in Section 3.2.

This numerical experiment was implemented with a computer running MATLAB® (The MathWorks Inc., 2013).

3.7. Preliminary assumptions and boundary conditions

In this section we have established the conditions that define the main characteristics of the C2C-CLMC system for this numerical experiment. The boundary conditions are key to the functionality of this model. Since in a C2C-CLMC system we are dealing with boundaries that are not naturally given by geometric motion of the volume of Si and it is not immediately obvious what these conditions are. Actual boundary conditions are more subtle. First, let R be region of the planet bounded by a closed curve with finite length (i.e. rectifiable curve) R_C . If Δx is known in R and x is given on R_C then the boundary conditions are prescribed in such a way that x is always known on R_C , and Δx is known in R , the solution of equation (16) (see Section 3) for the region R will be possible to determine. Therefore, since x is a function of time in R_C , velocity is known in the C2C-CLMC system. Consequently, the distribution of $\tilde{\rho}(x, t)$ after a ∂t will be known everywhere in R . Because of this, we may assert that the flow of Si is determined by the specification of x on the boundary, and the $\tilde{\rho}$ on that part of the boundary where the flow of Si is initially entering the interior region of R . Here, it is important to define the individual averaged units of $\tilde{\rho}$ through defining the quantities in the system. Density ($\tilde{\rho}_i$) is defined as the averaged units of $\tilde{\rho}$ per length at x_i and the flux ($\tilde{\rho}_i \tilde{u}_i$) is defined as averaged units of $\tilde{\rho}$ per time at x_i .

Some preliminary assumptions and boundary conditions have been imposed in this numerical test. This approach reduces computational burden of the simulation, time, and work efforts for large-scale system modeling, allowing for better performance of the entire numerical test. The preliminary assumptions and boundary conditions are displayed in Table 1.

The processing rate of averaged units of $\tilde{\rho}$ at each node ($\tilde{\xi}_n$) of the system (nodes 1, 2, 3, and 4 as shown in Fig. 1), is represented as a constant rate that is specific for each node since the processing rate is highly dependent on the technology available at each node. Therefore, in this experiment, due to the high uncertainty of processing rates at each node a heuristic argument is used to show that the following is probably correct: where the unit of $\tilde{\rho}$ is entering the area enclosed by the node, the $\tilde{\xi}_n$ must be imposed. The motion at every node is determined by the specification of $\tilde{\xi}_n$ everywhere on the boundary at which the volume of Si is entering the node. Based on the time scale already defined in this article (T_c), we have then estimated the order of magnitude for the constant processing rate for each node. The imposed values for $\tilde{\xi}_n$ are the following:

- For Node#1 and based on the definition of T_c , we have estimated T_{ind} based on our imposed manufacturing rate of 180,000 in one arbitrary year, we have estimated a value of $\tilde{\xi}_1 \sim 1 \cdot 10^{-2}$ units of $\tilde{\rho}$ per second.
- For Node#3, based on the data available from the Full Recovery End of Life Photovoltaic (FRELP) project (FRELP Project, 2018), it is estimated that in a recycling PV plant about 38 kg of Si can be recovered per hour. Since $\tilde{\rho}$ is known, we estimated the order of magnitude as $\tilde{\xi}_3 \sim 18 \cdot 10^{-3}$ units of $\tilde{\rho}$ per second.
- For Node#4, there is no ‘reservoir’ or similar infrastructure to extrapolate information or empirical evidence, therefore, we have estimated the magnitude of $\tilde{\xi}_4$ assuming that the magnitude of demand for recovered Si from the manufacturing solar and electronic industry is similar to the one from raw Si . We imposed the same order of magnitude at Node#1. Accordingly, $\tilde{\xi}_4 \sim 1 \cdot 10^{-2}$ units of $\tilde{\rho}$ per second.

Table 1
Summary of the assumptions and boundary conditions imposed in the numerical test

No	Assumptions and boundary conditions
1	In order to evaluate numerically the density flow of <i>Silicon</i> in a C2C-CLMC system at hemispheric scale, we have defined the following initial conditions: to reduce computational cost, we are only considering <i>Silicon</i> used in Photovoltaic panels as a single non-renewable natural primary resources in one-dimension (1-D).
2	All nodes are in a continuous processing system (24/7) with a 100% efficiency for each node. Except node-3, where recycling efficiency is imposed at the assumption number 4.
3	The manufacturing plant and distributors are subsidiaries of the same business group.
4	The recycling yield is imposed at 99%.
5	The PV panels are all manufactured according to Cradle-to-Cradle philosophy sufficient for the highest possible Cradle-to-Cradle certification and based on the elementary principles introduced in Section 3.2 to facilitate the disassembly phase. Hence, the Photovoltaic panels in question were designed to eventually be upcycled.
6	All returned <i>Silicon</i> is accepted for inventory either actively (moving directly back to the manufacturing process after the End-of-Life) or passively (at the reservoir, waiting to return to the manufacturing plant –depending on demand). Fig. 1 shows the corresponding nodes.
7	The entire Photovoltaic panel supply chain system is a vertically integrated and automated manufacturing facility. Since this numerical experiment is a test, for numerical simplicity we have imposed an input of 180,000 typical 250 Watt Crystalline-Silicone-Photovoltaic panels, assuming a 4.31 grams of <i>Silicon</i> per watt (Castellanos et al., 2018).
8	For the sake of simplicity, a maximal density function for Reservoir has been defined given by $\sum_i^n \bar{\rho}_i(t) [0, t] = [0, \max\{\bar{\rho}_i\}]$, (where $\bar{\rho}_i$ is the average material density at i), which is the maximum capacity allowed at the reservoir.
9	The length (L) of the C2C-CLMC system for a hemispheric scale has a typical value of about $L=4000$ kilometers (Contreras-Lisperguer et al., 2017). For this numerical experiment the distance between each node is assumed to be 1000 kilometers.
10	The initial boundary condition (IBC) for <i>Silicon</i> density is defined when the system is initially empty at $t=0$ (t =time) on the node-1, therefore, $\bar{\rho}(x, 0)=0$ ($\bar{\rho}$ =average density).
11	An averaged unit of density ($\bar{\rho}$) has been imposed as 1.5 kg of <i>Silicon</i> per Photovoltaic panel at x_i .
12	To minimize mathematical complexity, we have assumed the curvature of Earth neglected.
13	In this simulation we have used a suitable discretization with a uniform grid ($i\Delta x, n\Delta t$) with $i\Delta x = 10$ kilometers and with a total 404 space discretization points (101 per node). Thus, we have calculated the numerical stability of our model based on the selected Δx and Δt . The calculated stability condition is $\bar{u}_i \frac{\Delta x}{\Delta t} = 0.0003$. This satisfies the Von Neumann stability requirement described in Appendix D.
14	We consider a finite number of the average density ($\bar{\rho}$) of <i>Silicon</i> arriving in the system at $\bar{\rho}(0, t)$ for $t > 0$. Therefore, an arbitrary initial density inflow of <i>Silicon</i> entered the system. For this experiment a random initial input of $\bar{\rho}$ was chosen, initially 5 units of $\bar{\rho}$ entered the system, from a total of 180,000 units of $\bar{\rho}$ that entered the system at an average rate of 1000 unit of $\bar{\rho}$ per time step of the grid $\Delta t = \frac{0.0003 \cdot \Delta x}{\bar{u}_i}$ (Δt is estimated based on stability criteria described in Appendix D).
15	The flux of <i>Silicon</i> is a function of x and t and is determined by the average density ($\bar{\rho}$). Therefore, the flux can be defined as $\bar{\rho}_i \bar{u}_i$, where $\bar{\rho}_i$ is known and \bar{u}_i is a function of $\bar{\rho}$ and represents the averaged velocity of <i>Silicon</i> particles, and i represents the cell within the computational domain $\{1, 2, \dots, i\}$ for the periodic domain $x \in [0, L]$, where L represents the total length of the system. Consequently, the average velocity vector can be defined as $\bar{u}_i = \bar{u}_{(\bar{\rho}_i)} + \bar{u}_{(\bar{\rho}_{i+1})}$. Here, $\bar{\rho}$ propagates to the right on x .
16	The processing rate of averaged units of $\bar{\rho}$ imposed at each node ($\tilde{\xi}_n$) of the system are: $\tilde{\xi}_1 \sim 1 \cdot 10^{-2}$; $\tilde{\xi}_2 \sim 1 \cdot 10^{-9}$; $\tilde{\xi}_3 \sim 18 \cdot 10^{-3}$; $\tilde{\xi}_4 \sim 1 \cdot 10^{-2}$ units of $\bar{\rho}$ per second ($\bar{\rho}$ =average density).

- For Node#2, we have estimated T_d . The estimation of T_d is described in Appendix E.

4. Results and discussion

Given that for this numerical experiment T_d is approximately 30 years, as an initial test we performed a simulation of this C2C-CLMC system for 35 years ($\sim 1.1 \cdot 10^9$ s), illustrating a complete life-cycle of Si -flow described in Fig. 1. The goal of this simulation was to confirm that after 35 years the initial input of units of $\bar{\rho}$ returned to a manufacturing facility as raw material, fulfilling its purpose as a C2C-CLMC system. The resulting simulated profiles describing the flow of units of $\bar{\rho}$ in percentage per time for each node for this C2C-CLMC system are illustrated in Fig. 2.

As shown in Fig. 1, the flow of units of $\bar{\rho}$ are assumed to be 1-D flow. This data is useful for studying the time response of the material flow at each node (Fig. 2 - a, b, c and d) based on the conditions imposed in the numerical experiment. First, the raw material (initial input of Si units of $\bar{\rho}$) entered Node-1, where units of $\bar{\rho}$ are used to manufacture solar cells and become an integral part of a PV panel. As expected, the percentage of units of $\bar{\rho}$ decreased with time as manufactured PV panels left the manufacturing facility (see Fig. 2a) to be used in a power PV plant at Node-2. Then, at Node-2 the units of $\bar{\rho}$ increased up to the maximum $\bar{\rho}$ because they will be operational for about 30 years in a single place generating electricity at the PV plant (see Fig. 2b). Once the PV panel ends its operative life, the PV are decommissioned and sent to a recycling facility (Node-3), where Si units of $\bar{\rho}$ are recovered as raw material (see Fig. 2c). The recovered material is stored in the

“reservoir” (Node-4) and transported to the Node-1 as raw material (see Fig. 2d).

Based on data interpretation of Fig. 2a, it is possible that the flow of Si units of $\bar{\rho}$ was not able to return in its integrity to the manufacturing facility after the end of its operational life. We can see in Fig. 2a that at approximately $1 \cdot 10^9$ s, the system had retrieved less than 10% of the total Si units of $\bar{\rho}$ initially inserted in the system (see Fig. 2a). Here, we can conclude that the system was unable to close the material loop after one life cycle of 35 years.

Our initial hypothesis to explain this conundrum is to assume that the maximum $\bar{\rho}$ at Node-2 (see Fig. 2b) represents a critical convergence of units of $\bar{\rho}$ attributed to a large T_d . This triggered a shock wave that acted as a boundary between the high density observed at Node-2 and the low density observed at Node-3. The phenomenon is assumed to impact throughout the Node 3 and 4. This shock wave is reflected in a temporal variation of percentage of the units of $\bar{\rho}$ between Node 2 (high percentage of units of $\bar{\rho}$) and 3 (low percentage of units of $\bar{\rho}$), therefore, temporal variation of units of $\bar{\rho}$ requires spatial variation in the velocity \bar{u}_i , since continuity infers divergence of \bar{u}_i must be 0. Moreover, due to the continuous nature of the PV material flow, the shock wave can be identified because of the change in densities between the nodes that describes the boundary between two PV material flow states that are characterized by different densities, and flow rates. Therefore, it is possible to conceive that the shock wave moves in time and space disturbing the entire system, and limiting the flow of units of $\bar{\rho}$ to the Node-3, and restricting the capacity of the system to store Si units of $\bar{\rho}$ at the reservoir in Node-4. Consequently, the PV material flow was unable to close at Node-1.

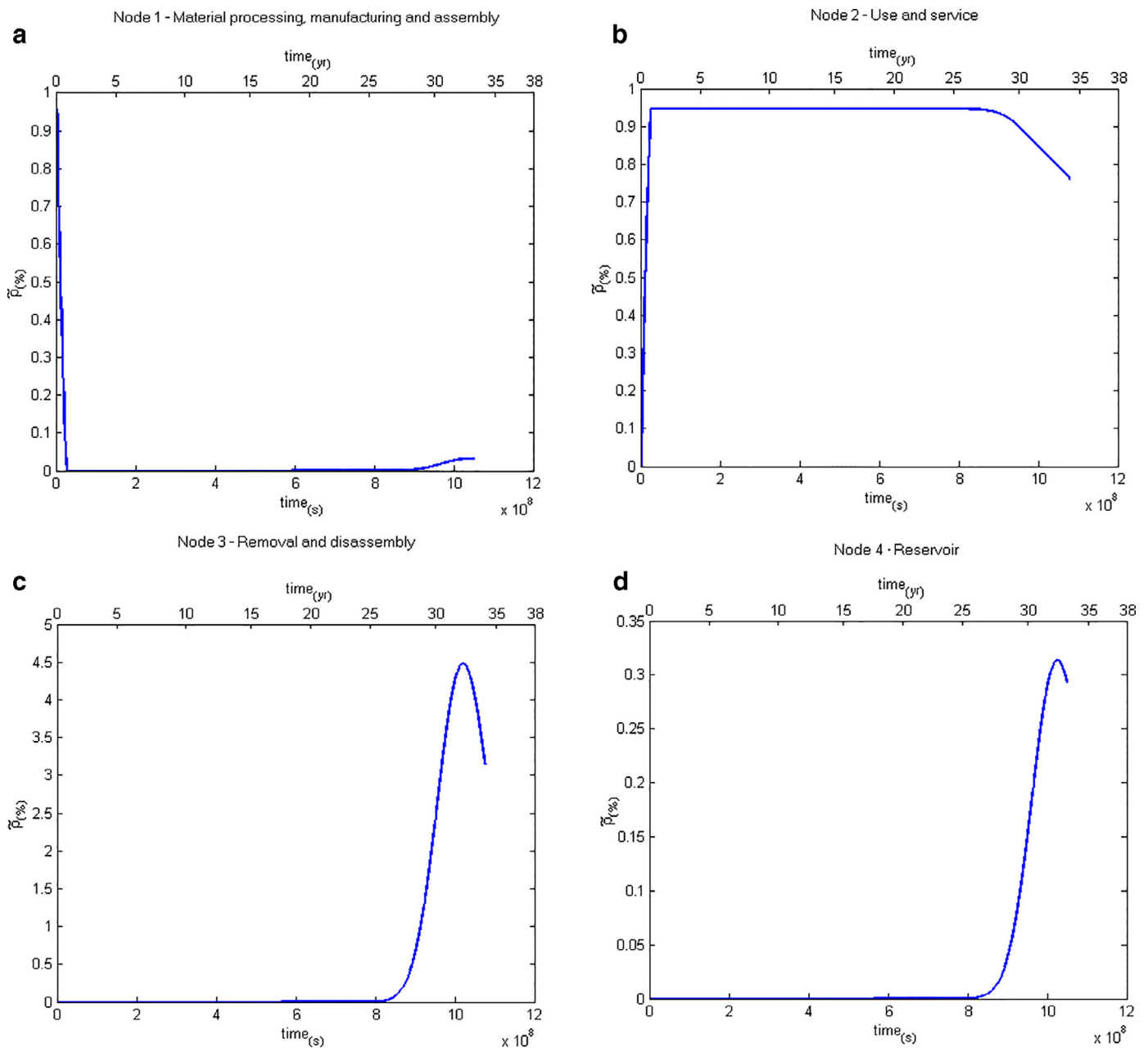


Fig. 2. Time series of the density percentage at each node from $t=0$ to $t=35$ years (on the top horizontal axis of the graph) and in seconds as standard international unit of time (SI) is on the bottom horizontal axis of the graph ($\tilde{\rho}$ = average material density, s =seconds, yr =years).

Another interesting feature observed in Fig. 2c and 2d is the “quasi-symmetry” in the distribution of $\tilde{\rho}$. However, we consider this a trivial symmetry due to the restriction imposed by the shock wave and the geometrical symmetry of the system modeled here. Additionally, the plots have different percentage of units of $\tilde{\rho}$ (see Fig. 2c and 2d), which leads us to believe this similarity can only be attributed to this test.

Applicability is clear from the previous results of our model since it provides a potentially useful approach to material flow simulation at hemispheric scale. Initial results have led us to question if the system will be able to close the material loop at any time in the future without introducing more new raw material into the system. In order to answer this question, and as a means of verifying initial findings and the consistency of the model, we ran a second simulation with the same conditions but for three cy-

cles totaling 110 years ($\sim 3.5 \cdot 10^9$ s). These results are presented in Fig. 3.

The results observed in Fig. 3 show the consistency of the model. The calculated flow of $\tilde{\rho}$ at each node (Fig. 3 – a, b, c and d) appear consistent with the previous results presented in Fig. 2.

Once the initial input of raw material (S_i units of $\tilde{\rho}$) entered Node-1 and when PV panels leave the manufacturing site, the percentage of units of $\tilde{\rho}$ decreased to zero, detailed in Fig. 3a. At $\sim 1.6 \cdot 10^9$ s (~ 45 years) it is possible to observe an input of material, around 25% of the total returned to the manufacturing facility (Node-1) as raw material. Finally, at $\sim 2.6 \cdot 10^9$ s (~ 80 years) the units of $\tilde{\rho}$ are constantly returning to Node-1, reaching the maximum return around $\sim 2.7 \cdot 10^9$ s (~ 85 years).

Like in the previous simulation, Node-2, $\tilde{\rho}$ increased to a maximum accumulation between $\sim 0.2 \cdot 10^9$ s (~ 5 years) and

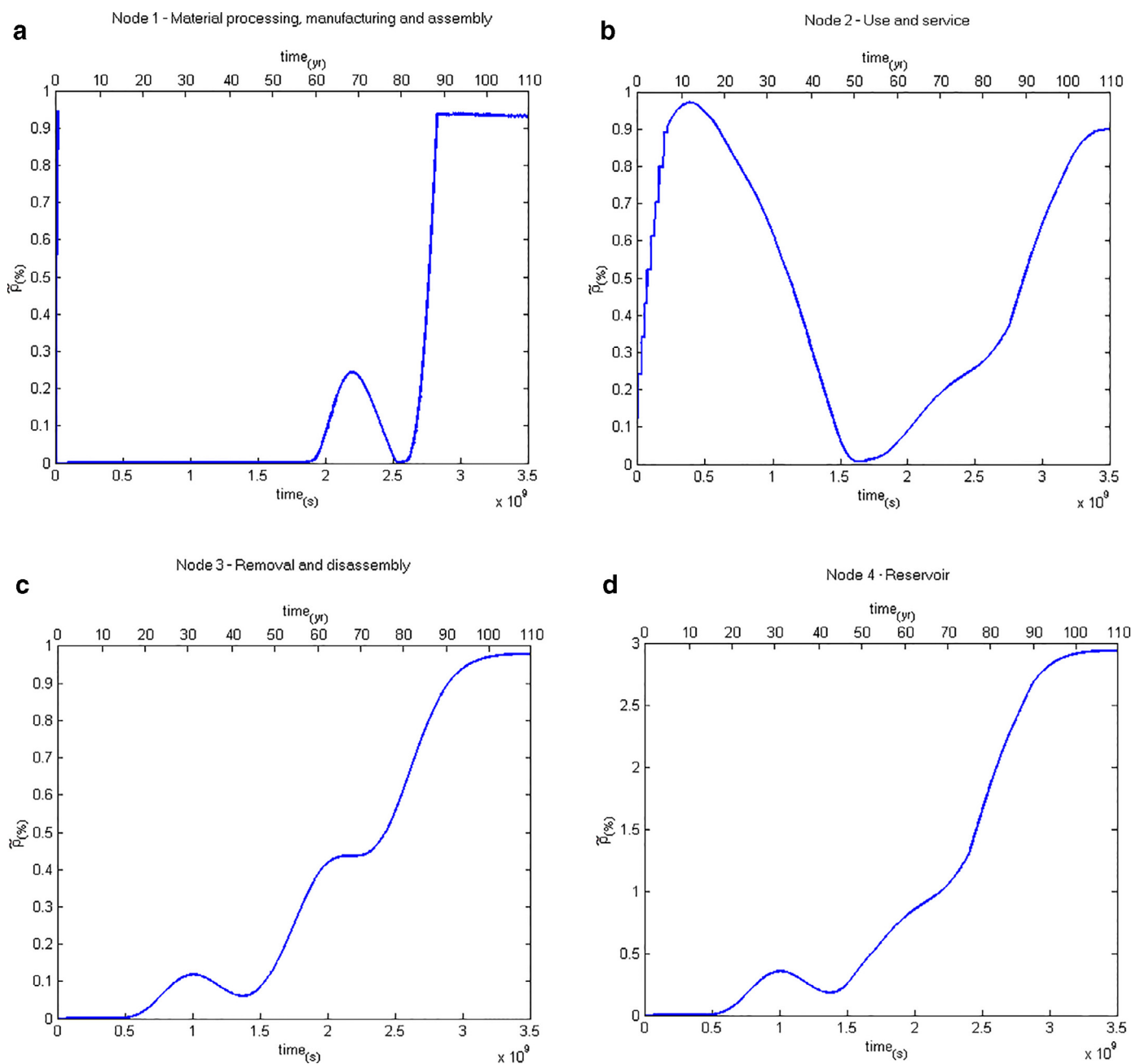


Fig. 3. Time series of the density percentage at each node from $t=0$ to $t=110$ years (on the top horizontal axis of the graph) and in seconds as standard international unit of time (SI) on the bottom horizontal axis of the graph ($\bar{\rho}$ = average material density, s =seconds, yr =years).

$\sim 1 \cdot 10^9$ s (~ 30 years), and then descend (see Fig. 3b). The high convergence of units supports our initial hypothesis about the impact of T_d on a closed system ($T_d \sim 29.949$ years in a fixed location generating electricity). Thus, we initially suggest that a large T_d creates an impact in the form of a shock wave that disturbs the C2C-CLMC system, causing it to reuse material ineffectively at EoL. This shock wave can be thought of analogously as a traffic jam, but instead of a red light or an accident that could last a couple of hours, PV panels are installed in a single place for 20-30 years or more with the sole purpose of generating electricity, causing an inertia that affects the entire closed system that can be seen in the results of our numerical experiments.

Continuing analysis of Node-2, we observe that at $\sim 1 \cdot 10^9$ s (~ 30 years, EoL for PV panel), the percentage of units of $\bar{\rho}$ start diminishing due to the decommissioning process of PV panels. Follow-

ing the trend observed in Node-3 (see Fig. 3c), we estimate that at $\sim 1 \cdot 10^9$ s (~ 30 years) the system was able to absorb around 25% of PV panels from Node-2, which is coherent with the amount of material reused at Node-1 (see Fig. 3a). Finally, at $2.8 \cdot 10^9$ s (~ 90 years) the system was able to reuse the total of units of $\bar{\rho}$ (Si material), gain stability, and close the material loop (see Fig. 3a).

For Nodes 3 and 4, we observed again a “quasi-symmetry” in the distribution of $\bar{\rho}$. However, the plots at Figs 3c and 3d are fairly different with a difference of several orders of magnitude, confirming our initial hypothesis.

As was shown in the results of this numerical experiment, the temporal evolution of $\bar{\rho}$ at each node initially suggests that a C2C-CLMC system at a global scale can be considered a system in steady-state, where the velocity of the material flow out of the Node regions can be faster than in it, which may be the result of

high momentum flow. However, the small momentum flow is also transported by the material flow once it is out of the Nodes. This is an important attribute of a C2C-CLMC system because recycling and upcycling cannot be instantaneous. Therefore, Node-4 plays a key role in helping the system reach stability after the shock wave triggered at Node-2, especially in cases where the recycling capabilities at Node-3 are limited. Consequently, Node-4 can provide a buffer capacity for the system, especially when non-pure or low-recyclable materials (e.g. highly random mixtures materials) are present in the system.

From the above results, some initial findings are drawn:

- 1 The numerical scheme used proves to be effective. The simulation is stable at T_d and able to provide a convergent solution for this simulation of Si flow during its entire life-cycle at hemispheric scale.
- 2 The model was able to effectively predict $\frac{\partial \bar{\rho}}{\partial t}$, the direction and magnitude of the material flow.
- 3 The model can reliably predict and identify a shock wave that affects the entire system. We initially suggest that T_d is the main culprit of this phenomenon.
- 4 Results show that the density (averaged units of $\bar{\rho}$ per length at x_i) behind the shock wave is different from the density ahead of the shock wave. This is why particles have enough time to experience delay under a steady process rate. Further research is needed to learn more about the shock wave propagation during material flow and the role of Node-4 (reservoir) in shock wave attenuation effects.
- 5 Although our simulations were originally implemented to evaluate the functionality and stability of our model, we initially believe our results can be considered a promising aspect for the implementation of a CLMC as a form of a CE system, contributing to the protection of the environment (Sauvé et al., 2016). Further analysis has to be done in terms of a real-time capable simulation.
- 6 The stability of the model and the successful numerical experiments performed show the encouraging performance of our model in capturing the dynamics of material flow at hemispheric scale. Promising initial results indicate the potential applicability of the proposed model to other complex physical systems at hemispheric and global scale at T_d .

Due to the non-linear nature of a CLMC system, as an alternative to the classic sensitivity analysis, a brief note using ensembles on the variations of T_d is included in the following section.

4.1. Simplified ensemble analysis

Though the uncertain aspects of our numerical model and its impact on a particular given set of assumptions have not been directly covered and are beyond the scope of this paper, our study does highlight the impact of T_d on the entire system.

A C2C-CLMC system is a non-linear system described by a set of differential equations. Since at least two first order systems exist in the series, two or more processes are equivalent to a second order system (Ingham et al., 2007). Therefore, our results agree with a higher-order nonlinear system. Changing the parameters within this specific system of operations has little impact on the results of the system (Forrester, 1987; Tjøstheim, 2012). So, for high-order non-linear systems, traditional linear sensitivity analysis may provide incorrect estimates (Saltelli, 1999).

Instead, we try to understand how a given uncertainty in T_d propagates throughout time in this dynamic system. In this research, we approach this question using the ensemble model framework. Ensemble model is an interesting statistical method that emerged in the last decade. It is used in many fields, such as: petroleum reservoir modeling (Jahanbakhshi et al., 2018), ocean

Ensemble Node 1 - Material processing, manufacturing and assembly

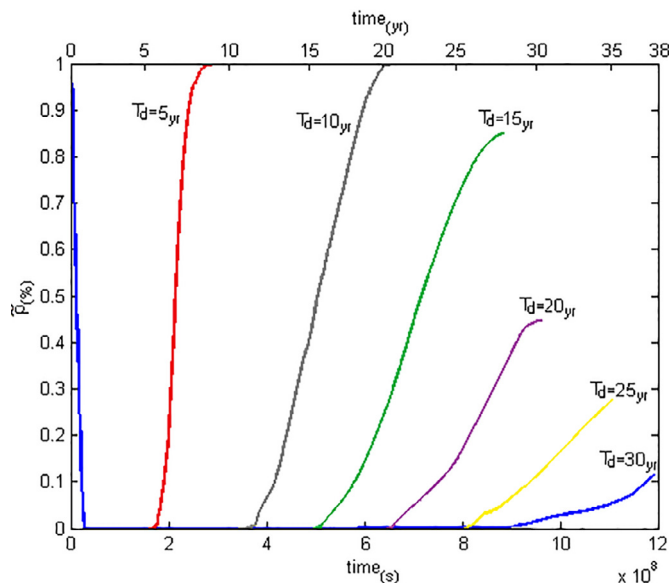


Fig. 4. Ensemble results for different dwelling time (T_d) (5, 10, 15, 20, 25, and 30 years), ($\bar{\rho}$ =average material density; s=seconds; yr=years).

dynamics (Nadiga et al., 2013), atmospheric science (Baran and Lerch, 2018), and hydrology (Seo et al., 2014), to name a few.

In this section, we use a simplified ensemble analysis to assess the sensitivity of a C2C-CLMC system at T_d . An ensemble model was constructed by running formulations of our model with different values for T_d (Fuentes and Foley, 2013). For this ensemble experiment, we ran a number of simulations for different T_d [5, 10, 15, 20, 25, 30] (years) at Node-1, where $T_d=30$ is our initial base-case scenario, then the ensemble results are compared to each other for $T_d=5,10,15,20,25$. Fig. 4 shows the results of the different profiles of $\bar{\rho}$ with time for each T_d .

The spatial variability in the distribution profiles of $\bar{\rho}$ at Fig. 4 evidences its dependency on T_d changes, confirming its key role for a closed PV panels system due to its large T_d . Moreover, the ensemble results show that an optimal T_d to effectively closed the material loop at hemispheric scale for a closed PV panel system is approximately between 5 to 10 years of operational lifespan. However, these initial results still need to be carefully interpreted and a more detailed study is needed.

5. Conclusions

This article has introduced a theoretical framework for CE in the form of a C2C-CLMC system, which was used for preliminary analysis of the dynamics for the PV material (Si) flow. This research has led to the following conclusions:

- We proposed and tested a numerical approach, which has been formally discussed to capture the dynamics of a PV material flow, introducing T_c , resulting in a stable model. Given the accelerated changes that the PV industry has experienced in recent years, we believe the strength of our model lies in its flexibility to be continuously updated to better capture the latest conditions deemed to be more representative of the moment.
- The numerical experiment has provided some initial insights into possible challenges related to the implementation of a CE system. Our initial findings shed some light on the limitation of closing the material flow for current C-Si PV panels if new raw materials are not introduced into the system.

- Preliminary ensemble results show a high dependence of the PV C2C-CLMC system on T_d , and a closed material flow cannot be achieved for T_d greater than 10 years.
- Our thermodynamic analysis suggests that in order to reduce waste generation at EoL and improve the sustainability in the solar PV sector, the industry will need to avoid the use of inter-mixed materials typically found in C2G products. Consequently, if C-Si PV panels contain consistently high-grade, non-random mixtures, less work will be required to recycle a PV panel.

Future research activities should aim to study the material flow for C-Si PV using real-time data provided by different PV stakeholders. Adapting the parameters of the model using real-time data accordingly will help us better understand the dynamic of different manufacturing processes, supply chains, and recycling technologies. Although high-performing computer resources will be needed to conduct these studies, they could very well pave the way for a CE in the entire PV industry. Moreover, future research should aim to study the material flow for other PV technologies by applying different boundary conditions and parametrizations. Lastly, we suggest that the combined use of our model, in conjunction with tools such as LCA, can guide implementation of the CE concept in the PV industry. This way, industry leaders will be able to explore the potential economic benefits of reducing the operational life of a C-Si PV panel, design more sustainable policies, create social awareness, and improve infrastructure that is needed to transform today's fundamentally linear economy. Despite these points, a transparent process is necessary to ensure integrity and to afford stakeholders the opportunity to make informed decisions, otherwise, a CE model based on a C2C-CLMC system per se will not guarantee long-term sustainability.

To the best of our knowledge, our study is among the first of its kind that integrates a material-flow dynamic model based on PDE, introduces the concept of circular time, and uses thermodynamic analysis for theoretical material flow (Si) in the PV industry on a hemispheric scale. The results presented are promising and can be useful to other industrial sectors.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Supplementary materials

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Linear versus Circular: Cradle-to-Grave and Cradle-to-Cradle

Cradle-to-Grave

Cradle-to-Grave (C2G) is the current prevailing paradigm in the manufacturing sector and the entire supply chain system. The solar photovoltaic (PV) sector promotes inefficient recovery of residues

and waste at End-of-Life (EoL) due to the linear lifetime of crystalline silicon photovoltaic (C-Si PV) panels. Since the extraction of material (*cradle*) is considered waste (*grave*) until EoL, only a small portion of the materials reach the “recycling phase” where most of the panels were not designed for recycling purposes or to be reused at the EoL (Fig. 5). Here, the C2G process exemplifies “down-cycling”:

Today, eco-efficiency principles provide a degree of environmental relief, along with certain economic benefits. Nevertheless, there is still a lack of a fundamental redesign of material flows and inadequately addresses the level of toxicity in some products (Braungart et al., 2007). Furthermore, there is no clear evidence, either historical or theoretical, that efficiency improvements will decrease the amount of resources used (Smil, 2008). Eco-efficiency can, however, be considered a link between current C2G paradigm to a new circular paradigm.

Cradle-to-Cradle

The cradle-to-cradle (C2C) philosophy was introduced in the book *Cradle-to-Cradle: Remaking the Way We Make Things* (McDonough and Braungart, 2002). Products are designed and engineered to avoid toxicity to the environment, not just during their manufacture process, but over the full course of their useful life, while also making it possible to reutilize their materials at the EoL (McDonough and Braungart, 2002). The entire lifecycle of a C2C product mimics a circular industrial system, where all materials can be potentially used and reused indefinitely. Hence, the materials used to manufacture a PV panel or any other product at the EoL can be upcycled as a primary resource to manufacture the same product or a different one (Fig. 6).

The C2C is based on three main principles (McDonough and Braungart, 2002):

- Waste equals food;
- Use current solar income;
- Celebrate diversity.

These main principles can be divided more comprehensively based on the C2C certification program (McDonough Braungart Design Chemistry, 2012). The five principles are:

- *Safe Materials*: products are designed with non-toxic materials.
- *Reutilization (upcycling)*: used in a closed-loop-cycle where all materials flow indefinitely in cycles.
- *Water*: Water control in the industrial process and the effective use of it. In-flow and out-flow of water is purer during the industrial process.
- *Energy*: Maximize use of renewable energy sources and technology. Energy is effectively used (Improve Energy Efficiency by Cascade Effect use on Industrial Systems).
- *Social fairness*: social impacts of C2C approach must be improved in terms of existing social conditions and future planning and design, always considering local conditions where industrial facilities operate.

In a circular flow of mass, C2C defines two cycles or *metabolisms* depending on types of materials used in production: the biological and technical cycles. The biological cycle illustrates the life cycle of manufactured products that use exclusively biodegradable materials such as cotton, paper, or wood, among others, that can be considered biological nutrients (McDonough and Braungart, 2002). Since PV panels are not made with these materials, we do not discuss this cycle in the paper. The **technical cycle** (see Fig. 6), as defined by the C2C philosophy, is the life cycle where material flows in circles, where all adequately selected materials are used and then reused as raw material into the industrial system (McDonough and Braungart, 2002). The C2C

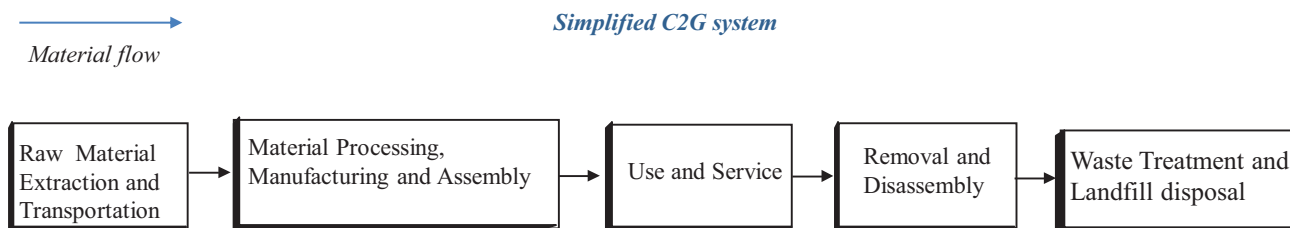


Fig. 5. Cradle-to-grave: Simplified linear flow of materials (adapted from Contreras-Lisperguer et al. 2017)

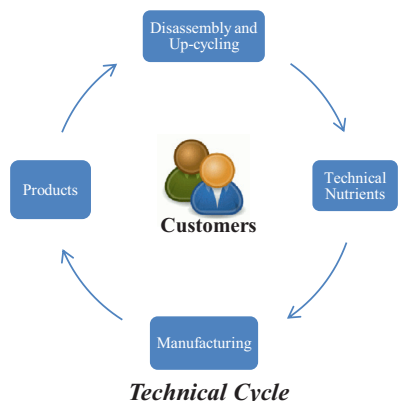


Fig. 6. Cradle-to-cradle: Technical cycle (adapted from Contreras-Lisperguer et al. 2017)

philosophy promotes an eco-effectiveness by creating an industrial material flow like what happens in nature, where the use of materials is safe and healthy for the ecosystem, and there are materials flowing within different cycles, increasing the overall system efficiency (Braungart et al., 2007).

C2C practitioners assert that the Life Cycle Assessment (LCA) tool is not suitable to assess the “C2C-ness” of a C2C-product (NL Agency, 2011), therefore, C2C Certification™ (MBDC LLC., 2012) is the only available tool to assess a C2C-product and is implemented by the Cradle-to-Cradle Products Innovation Institute (Cradle to Cradle Products Innovation Institute, 2017). However, as others have mentioned, this exclusionary approach for the C2C Certification scheme is questionable (Llorach-Massana et al., 2015) an LCA tool may actually complement C2C certification (Toxopeus et al., 2015).

The certification has five categories (Basic, Bronze, Silver, Gold, or Platinum), representing levels of accomplishment and adherence to prescribed requirements for each category.

C2C philosophy has not only gained popularity in the manufacturing sector, but also garnered attention from critics. Based on the available scientific literature, most of the critics are focused on the C2C Certification™ scheme. Llorach-Massana et al. 2015 and Bach et al. 2018 point out that the C2C Certification™ does not consider the environmental impacts of a C2C-product from a life cycle approach and focuses mostly on the raw materials and end of life stages. Meanwhile, Toxopeus et al. 2015 highlights that the C2C Certification™ mainly focuses on material health, with the category material reutilization a distant second, and the aspects of water stewardship, renewable energy, and social fairness are implemented and assessed far less extensively. Other literature focuses on the benefits that LCA and eco-efficiency practitioners could gain from the C2C philosophy regarding the importance of resource efficiency and positive environmental effects from materials. Furthermore, de Pauw et al. 2015 stressed that LCA methodology must expand its boundaries in order to assess sustainability and main impacts from nature-inspired design products (i.e. C2C

and biomimicry). Some authors underline the need to address conflict between sustainability, unlimited growth, and consumption by focusing on eco-effectiveness along with the traditional focus on eco-efficiency in our industrial development (Hauschild, 2015).

It is possible to conclude that the C2C philosophy has an important value by helping to the establish foundations under which this CLMC system will be designed.

Dwelling time estimation

Dwelling time (T_d) represents the time that materials remain in operation or with the consumer before being reintroduced as a primary resource into the manufacturing cycle. T_d equals the time-frame between (a) the start of use and service and (b) removal or recovery. In reality, the operational lifespan of C-Si PV panels can only be approximated by mathematical models (e.g. trend analysis, probabilities, etc.). For C-Si PV panels, T_d is assumed to be closely related to the operational lifespan until C-Si PV panel failure. This assumption facilitates estimation while fundamentally satisfying the definition of T_d .

With this said, T_d can be represented as a continuous non-negative random variable that has a probability density function (pdf) denoted by $f(t)$. The cumulative distribution function (cdf) of $F(t)$ is then the integral of pdf. Here, $F(t)$ represents the probability that a system will be functional in the interval from time 0 to time t , and can be written as:

$$F(t) = P(T_d \leq t) = \int_0^t f(s) ds \text{ for } t \in \mathbb{R}^+ \tag{B.1}$$

In the case of C-Si PV panels, T_d amounts to the time from when the typical C-Si PV panel starts operation -generating electricity- until the same panel is no longer functional. Thus, using equation (B.1) it is possible to express the reliability function (Mishra and Joshi, 1996) as:

$$R(t) = 1 - F(t) = P(T_d > t) \text{ for } t > 0 \tag{B.2}$$

where $R(t)$ in equation (B.2) represents the probability that the PV panel is still working at time t and can be considered as a proxy of the average lifetime of a PV panel. Based on reliability theory (Ross and Ross, 2019) it can be written as follows:

$$T_d = \int_0^\infty R(t) dt \tag{B.3}$$

Conservation of mass equation and its linearization

As an initial approximation, let us assume that the flow of mass of Non-Renewable-Abiotic-Primary-Resources (NRAPR) at any time-space scale and at any manufacturing phase observed at T_c will behave as a continuum rather than as discrete particles. Our initial assumption can be seen as an extension of symbiotic industrial material flows through the networks of different businesses at different time-space scales (Chertow, 2004). Let's consider an

imaginary finite NRAPR volume with dimensions $\delta x, \delta y, \delta z$, containing a fixed collection of matter displaced across a field property $\varepsilon(x, y, z, t)$ through any arbitrary manufacturing phase. As the system is comprised of a fixed collection of matter, the shape of the finite volume of material (NRAPR) will be distorted by the various forces applied during the manufacturing processes. However, since the density is unchanged over time, we can write the conservation of mass equation as:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho Y) = 0 \tag{C.1}$$

Equation (C.1) is the Euler form of a first-order hyperbolic equation (Craig, 2013), which describes the mass-conservation equation for given bodies of NRAPR, where ρ represents the NRAPR or material density in terms of ρ per units of length and Y represents the three-dimensional velocity vector. One more step is needed to comply with our first assumption that at any time and space scale, the flow of a mass of NRAPR observed at T_c can be considered continuous. Since material flow happens at different time and space scales (Contreras-Lisperguer et al., 2017), it has both an average and a fluctuating component. Therefore, we shall now derive the conservation of mass equation in its averaged form. To avoid unnecessary complexities, we opt for the Favre approach over the Reynolds approach (Ruffin et al., 1997).

After decomposing the variables into a mass-weighted mean and the fluctuating part (non-linear), we apply Favre decomposition of the motion field in (1) and obtain the Favre time averaged conservation of mass equation:

$$\frac{\partial \tilde{\rho}}{\partial t} + \tilde{Y} \nabla \cdot \tilde{\rho} = 0 \tag{C.2}$$

Where $\tilde{Y} = \tilde{u}_i + \tilde{v}_j + \tilde{w}_k$ represents the average three-dimensional velocity vector at every stage of the life-cycle of a product. Equation (C.2) allows only for the determination of mean quantities at a global/regional scale, which may differ from instantaneous ones. We shall now use a numerical scheme to solve this differential equation.

Stability analysis of our model

A stable numerical scheme is crucial to successfully modeling the C2C-CLMC system. It can be considered stable if any numerical errors generated during the solution of discretized equations are not amplified (LeVeque, 1992). Since equation (17) is a linear finite-differential equation with constant coefficients (Durrant, 2010), we have used Von Newman Stability analysis to assess the stability of the scheme. We considered a single Fourier component in order to examine the growth of the error in time on an individual harmonic of the form

$$\psi_i^n = \psi(x_i, t_n) = \alpha^n e^{i\theta i \Delta x} \tag{D.1}$$

where α is the amplification factor. The numerical scheme is unstable if $|\alpha| > 1$. Hence, for stability we need to satisfy the requirement

$$|\alpha| \leq 1$$

If we then introduce ψ_i^n on our numerical scheme equation (D.1), then, we can rewrite (D.1) as

$$(\alpha^{n+1} - \alpha^n) e^{i\theta i \Delta x} + \nu \alpha^n (e^{i\theta i \Delta x} - e^{i\theta (i-1) \Delta x}) = 0 \tag{D.2}$$

where $\nu = \tilde{u} \frac{\Delta t}{\Delta x}$

Removing powers of α and using $e^{i\theta i \Delta x}$ as a common factor gives

$$\alpha = 1 - \nu + \nu e^{i\theta \Delta x} \tag{D.3}$$

Then, by applying the exponential form identity we can rewrite α as

$$\alpha = 1 - \nu + \nu (\cos(\theta \Delta x) - i \sin(\theta \Delta x)) \tag{D.4}$$

We can find the magnitude of α by taking the square root of the multiplication of α per its complex conjugate α^*

$$|\alpha| = \sqrt[2]{\alpha \alpha^*}$$

Consequently,

$$|\alpha| = 1 - 2\nu + \nu^2 + 2\nu \cos\theta - 2\nu^2 \cos\theta + \nu^2 \cos^2 + \nu^2 \sin^2 \tag{D.5}$$

$$|\alpha| = 1 - 2\nu(1 - \cos\theta) + 2\nu^2(1 - 2\cos\theta) - 1 + 2\nu(1 - \cos\theta)(\nu - 1) \tag{D.6}$$

Simplifying the trigonometric expression (D.6) using trigonometric identities, we have

$$|\alpha| = 1 + 4\nu(\nu - 1) \tag{D.7}$$

Thus, equation (D.7) only satisfies the stability criteria, if and only if $\nu \leq 1$ then, $|\alpha| \leq 1$.

$$|\alpha| = 1 + 4\nu(\nu - 1) \leq 1 \tag{D.8}$$

Since $\nu \leq 1$ is sufficient to demonstrate a condition of stability and $\nu = \tilde{u} \frac{\Delta t}{\Delta x}$, then, the Von Neumann stability condition is in the form of the Courant–Friedrichs–Lewy (CFL) condition, as

$$\tilde{u} \frac{\Delta t}{\Delta x} \leq 1 \tag{D.9}$$

and a non-negative Δt and Δx denotes

$$\tilde{u} \frac{\Delta t}{\Delta x} \geq 0 \tag{D.10}$$

in order to satisfy both conditions (D.9) and (D.10), we can rewrite the stability condition as

$$0 \leq \tilde{u} \frac{\Delta t}{\Delta x} \leq 1 \tag{D.11}$$

Our experiment must satisfy (D.11) to be considered stable and the satisfactory simulation.

Estimating Dwelling time for a crystalline silicon photovoltaic panel

To estimate Dwelling time (T_d), we considered that the degradation and failure of a PV panel can be represented by a Weibull function (Charki et al., 2013; Pregelj et al., 2001). This function represents the T_d distribution for C-Si PV panels in the form

$$f(t) = \left(\frac{\alpha}{\beta}\right) \left(\frac{t}{\beta}\right)^{\alpha-1} e^{-\left(\frac{t}{\beta}\right)^\alpha} \tag{E.1}$$

where,

$$F(t) = P(T_d \leq t) = \begin{cases} 1 - e^{-\left(\frac{t}{\beta}\right)^\alpha} & \text{for } t > 0 \\ 0 & \text{otherwise} \end{cases}$$

then,

$$R(t) = e^{-\left(\frac{t}{\beta}\right)^\alpha} \quad t > 0 \tag{E.2}$$

By applying equation (E.2) over (E.1), it is possible to estimate T_d

$$T_d = \int_0^t R(t) = \beta \Gamma\left(1 + \frac{1}{\alpha}\right) \tag{E.3}$$

Then the mean T_d may then be written as follows

$$\bar{T}_d = \beta (\ln 2)^{\frac{1}{\alpha}} \tag{E.4}$$

For this numerical experiment, the estimation of parameters α and β were made based on statistical methodologies and random failure sample (Pregeelj et al., 2001; Ramadan, 2015) using the Weibull reliability toolkit for R (Weibull-based reliability toolkit for R, 2013), then, the parameters found for this particular experiment are $\alpha = 5.376$ and $\beta = 32.062$.

Introducing α and β on equation (E.4), we obtain $T_d = 29.949$ years $\approx 9 \cdot 10^8$ s, which matches the average lifecycle of a typical PV module. Since T_d and $\tilde{\rho}$ are known, we estimated that the order of magnitude of $\xi_2 \sim 1 \cdot 10^{-9}$ units of $\tilde{\rho}$ per second, which represents the decommissioning rate of units of $\tilde{\rho}$ once the PV panel is no longer functional.

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