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# Quantification of the Inconvenient Truths about the Circular Economy (CE)

## Digital Twinning of Very Large Systems

*We discuss the limitations to material flows from recycling in the circular economy, using as a case the simulation-based analysis of the CdTe Photovoltaic cells. It is important to use a simulation basis for the analysis, since this permits the quantification of all material losses both in terms of exergy and energy simultaneously i.e. 1st and 2nd law of thermodynamics. Harmonizing this with the power supply flowing into the system and minimizing energy usage as well as exergy losses will maximize the resource efficiency.*

### What is the Circular Economy (CE)?

The Circular Economy (CE) concept has the noble objective of transforming economies from linear to circular models in which waste materials (traditionally reporting to landfill) are returned and utilized as resources as far as possible. The CE concept has excellent and important intentions: to stop or reduce the anthropological damage inflicted upon our planet and to ensure its future habitability. At its core lies the efficient use of all resources e.g. human, natural and economic. (Beaulieu et al. 2015, Reuter et al., 2019)

The Ellen MacArthur Foundation (2017) defines the Circular Economy (CE) as

> *"Looking beyond the current 'take, make and dispose' extractive industrial model, the circular economy is restorative and regenerative by design. Relying on system-wide innovation, it aims to redefine products and services to design waste out, while minimising negative impacts. Underpinned by a transition to renewable energy sources, the circular model builds economic, natural and social capital."*

However, when translating this significant message to images, it is striking that neither the key extractive industry nor energy and exergy i.e. key physics laws that describe the variability of the CE system are depicted. While the Ellen MacArthur definition of a CE economy directs a torch and illuminates its many dimensions, ultimately the economic viability of the CE, as would be the case for any economically viable processing system, requires a deep understanding of all the losses, environmental impact and associated risks from the system. These must be understood simultaneously and subsequently be quantified economically to ensure materials stay in circulation as long as possible with the required material quality. The laws of physics must form the DNA of all the formulations and simulation models *(digital twins)* that describe the very large complex and interconnected systems of the CE.

The EU's Green Deal (2020) is an innovative leader and its action plan is pushing strongly towards circularity; a very commendable action of the European Union (EU). While the EU's document speaks various times of energy, it neglects to speak about exergy (entropy) and the resulting inevitable losses from the CE system. These losses contribute significantly to the economic performance of the complete complex and interconnected system (Verhoef et al. 2004; Reuter et al., 2019).

The EU's document embraces among others the CE definition of Kirchherr et al. 2017

> *"A circular economy describes an economic system that is based on business models which replace the 'end-of-life' concept with reducing, alternatively reusing, recycling and recovering material in production/distribution and consumption processes, thus operating at the micro level (products, companies, consumers), meso level*

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*(eco-industrial parks) and macro level (city, region, nation and beyond), with the aim to accomplish sustainable development, which implies creating environmental quality, economic prosperity and social equity, to the benefit of current and future generations."*

Essentially this definition encapsulates according to its authors, CE's core principles: the 4R framework (reduce, reuse, recycle, recover), waste hierarchy, and a systems perspective; its aims: Sustainable Development (SD) resulting in environmental quality, economic prosperity and social equity, now and into the future; and its enablers: business models and consumer consumption behavior (Kirchherr et al. 2017, Jawahir et al. 2006, Blomsma and Brennan 2017, Beaulieu et al. 2015, Homrich et al. 2018, Lansink 2017, Lieder and Rashid 2016). Furthermore, the CE embraces green economy, functional economy, industrial ecology, shared value, extended producer responsibility, ecodesign and *cradle-to-cradle* thinking, amongst others. The United Nations *Sustainability Developments Goals (SDGs)* elegantly incorporate so many of these positive developments (*https://sustainabledevelopment.un.org/?menu=1300*). Lieder and Rashid (2016) identify nine fields that have to link in supply chain i.e. industrial ecology, environmental science, economics, business management, supply chain management, sustainability science, process engineering, law and policy, as well as social science to harmonize activities in the complete supply chain. This requires an open communication between these fields (Ghisellini et al. 2017, Jackson et al. 2014) to realize a flow of material, energy, and goods with the least possible losses (Abadías et al. 2020).

How these losses can be estimated to analyse the performance of the CE system we will discuss in the following section. This gleans from a recent interview by Reuter (2019) entitled *Design for Recycling – Inconvenient truths of the circular economy*.

## The required detail to understand the circular economy

A meaningful analysis of the CE can only be made if a detailed understanding is available of the flow of all materials and their embodied latent energy through the very large systems of the CE. First of all, fundamental thermodynamic data must be available for all the materials so that their energy flows can be estimated. Most importantly the dissipation of *exergy* (increase of entropy) from the CE system – all streams are in fact energy flows. This makes the use of process simulation tools an imperative to perform the fundamental analysis and economic optimization of the complete system that is depicted by Figure 1. This provides the rigorous process-engineering analysis and basis that enables the linkage of all the stakeholders of the CE system as detailed by Figure 1. This analysis underpins the complete supply chain from the resource to the final product, including the product design and *End-of-Life (EoL)* treatment on physics-based foundation e.g. through the exergy dissipation from the system as depicted by Figure 1. This permits the linkage of the energy flow in the materials with the energy grid and power supply, harmonizing the resource efficiency and quantifying it in units of energy flow i.e. MWh/h or MJ/h.

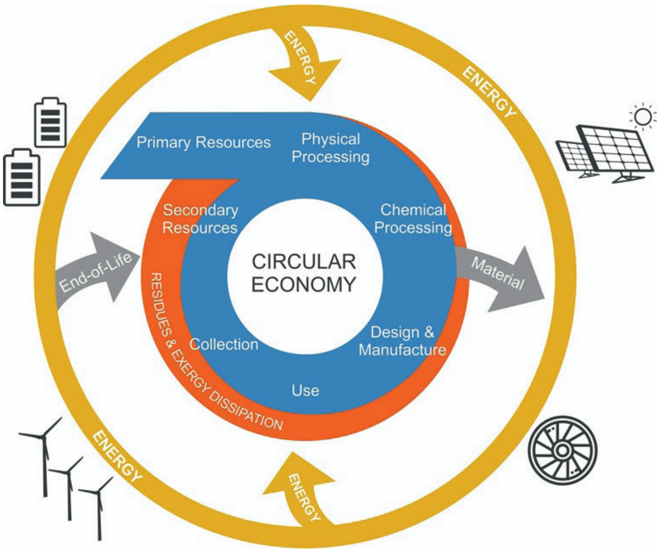


*Figure 1: The CE – Key challenge to harmonize the renewable energy and processing industries through digitalization to quantify and optimize resource efficiency on a fundamental basis (Abadías et al., 2020).*

Revealing the complexity of the enabling process metallurgy infrastructure of the CE is important for optimizing its performance and thence quantifying the losses as depicted by the outer spiral in Figure 1 (*Residues and Exergy Dissipation*). Therefore, to illustrate the (in)compatibility of metals and materials, which is a significant driver of recovery and losses of metals that are functionally combined in product design, the Metal Wheel was developed (Figure 2). The objective of this specific depiction is to show in a concise manner which metals and their minor metals are recovered through the shown carrier metals production (centre band) and the inevitable losses from the system due to its chemistry and technology infrastructure and metals that are connected in design (the outside band).

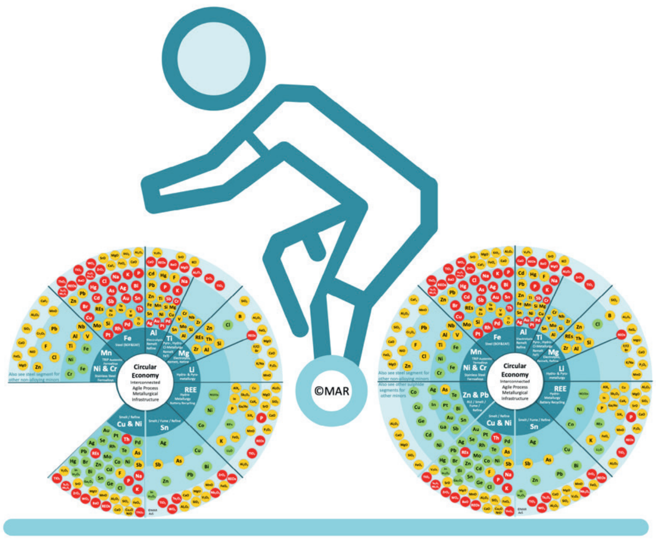


*Figure 2: The Metal Wheel (back) depicting various losses (outside band) and economic recoveries of technology elements (two middle bands) on the back of various critical carrier metallurgical systems (inside bands) (Verhoef et al. 2004). Removing segments from the wheels (front wheel) i.e. carrier metallurgy infrastructures has catastrophic results for the CE (Blanpain et al. 2019, Reuter et al. 2019).*

In summary Figure 1 supported by Figure 2 implicitly and elegantly link energy, entropy (thus exergy), product and geological mineralogy, product design and extractive industry to the losses from the CE. The above detail knowledge has been available for many years, summarized by the UNEP report on Metal Recycling (UNEP, 2013). Unfortunately, Ciacci et al. (2015) still attempt to discuss the dissipation of elements without considering thermodynamics and complex interactions. With the detailed analytical tools available it is, however, possible to show the true losses from intricate products (Reuter, 2016). Especially for the dilute elements a large amount of energy (and associated entropy creation) would be required to recover them from complex solutions, complex products, alloys, material combinations etc. to create once again high-quality functional materials, their combinations and alloys that deliver the performance and functionality of modern technology. The work of Mendoza et al. (2017) hardly reaches a depth that enables the evaluation of the CE on a rigorous basis at a level of detail that allows for the effects of redesigns on systemic losses to be estimated. So often, fundamental aspects are still missing in many of the CE documents mentioned above and special editions of journals such as the *Journal of Industrial Ecology* with the editorial by Bocken et al. (2017). They do not critically discuss the limits of the material and metal processing system in a sufficiently fundamental manner. The word entropy hardly appears in the 20 or so papers in this special edition on CE. This thermodynamic quantity that makes losses unavoidable, is not mentioned and neither fully understood in the context of economic feasibility of the CE nor in the context of the phrase *closing the loop.* Nor is detailed simulation analysis of the intricate and very large system based on fundamental understanding discussed. Fact of the matter is that no recycling loop can ever be fully closed!

In summary: There are large and significant knowledge gaps that challenge the optimization and also the digitalization of the CE i. e. also linking the energy and resources system together, to estimate the true losses (Reuter 2016). Therefore, we will very briefly show how such detail can be captured in digital twins of large CE systems.

## The digital twin of large-scale CE systems and their analysis

The software platforms that can describe the large systems of the CE have been developed over numerous years (see Reuter 1997, Reuter and Van Schaik 2012, Bartie et al. 2020, Abadías et al. 2020, Fernandes et al. 2020) and have been commercially realized in the simulation software *HSC Sim 10* (Outotec 2020). Into the HSC Sim software tools have been incorporated such as:

- *Life Cycle Assessment* (LCA) analysis tools that permit a direct export of all simulated results to *GaBi* (*https://sphera.com/product-sustainability-life-cycle-assessment-lca-software/*) and *openLCA* (*http://www.openlca.org*) and

- detailed thermoeconomics tools that permit the detailed exergetic analysis of these large systems (Abadías et al., 2019).

Numerous cases have recently been completed to fully understand the CE, of which the following are a short summary:

- Mobile phones and the effect of modular design on circularity and resource efficiency (Fairphone 2018). A recyclability index has been developed and applied to visualize in a simple manner the recyclability of products.

- Linking of the complex resource system from mine to metal and NdFeB magnets to their end-of-life and back into magnets (Fernandes et al. 2020).

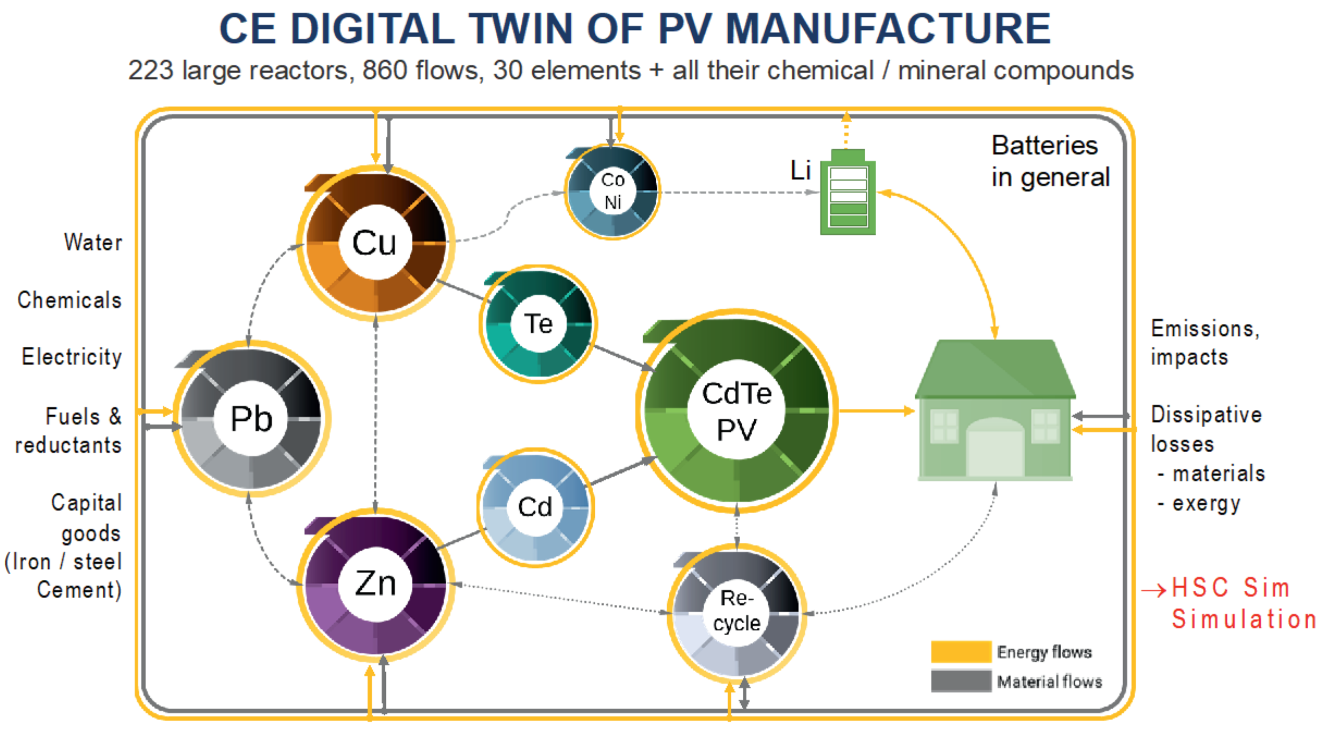


*Figure 3: The complex metallurgical infrastructure that produces the metals and residues to produce CdTe photovoltaic (PV) cells showing the nexus energy and materials connected using process simulation tools. (Bartie et al. 2020)*

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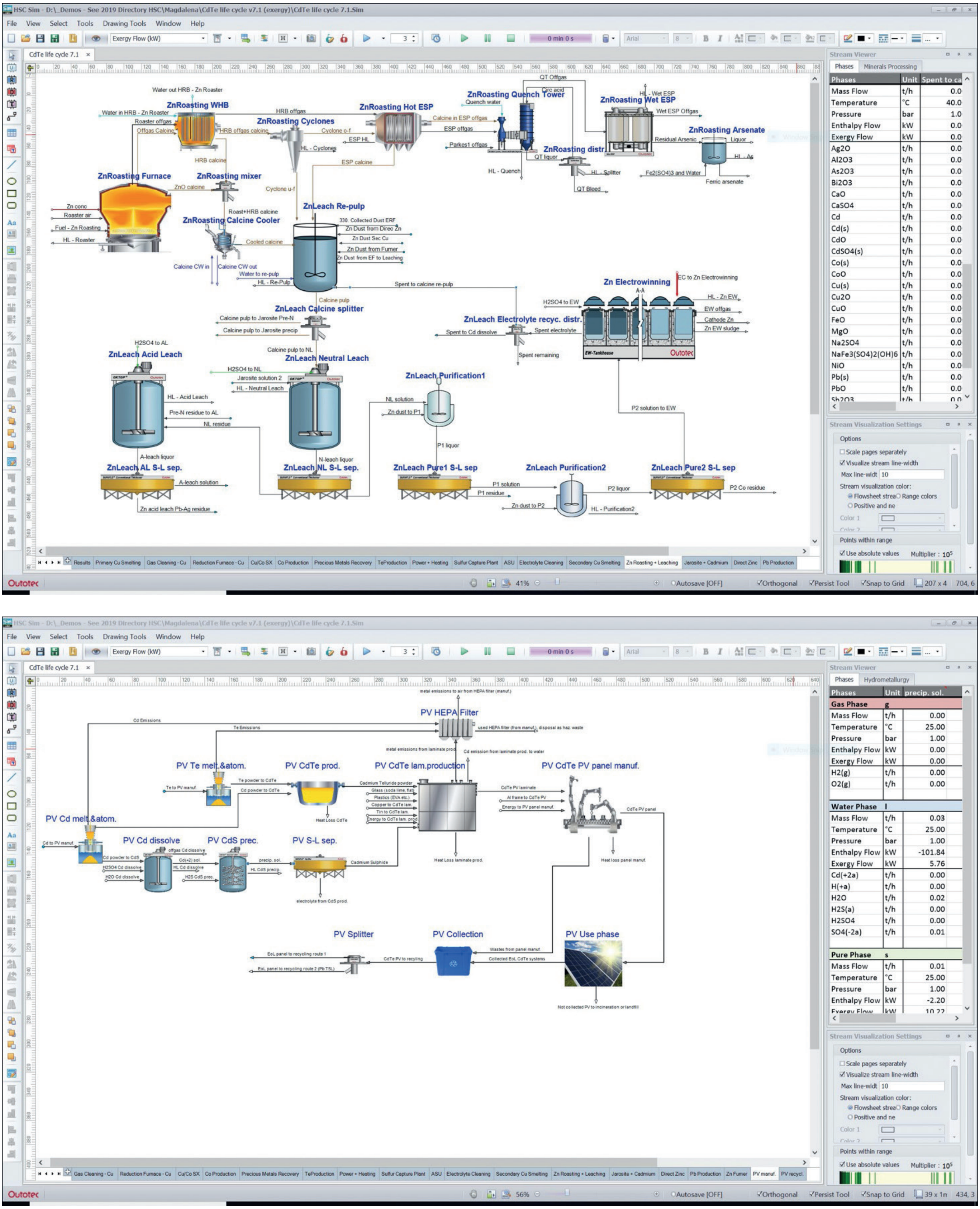


*Figure 4: HSC Sim simulation model representing Figure 3, two of 19 simulation panes of the complete system are depicted (Abadías et al. 2020, Bartie et al. 2020) – the top figure depicting the model for primary zinc carrier process metallurgy and the bottom figure showing the PV cell manufacturing.*

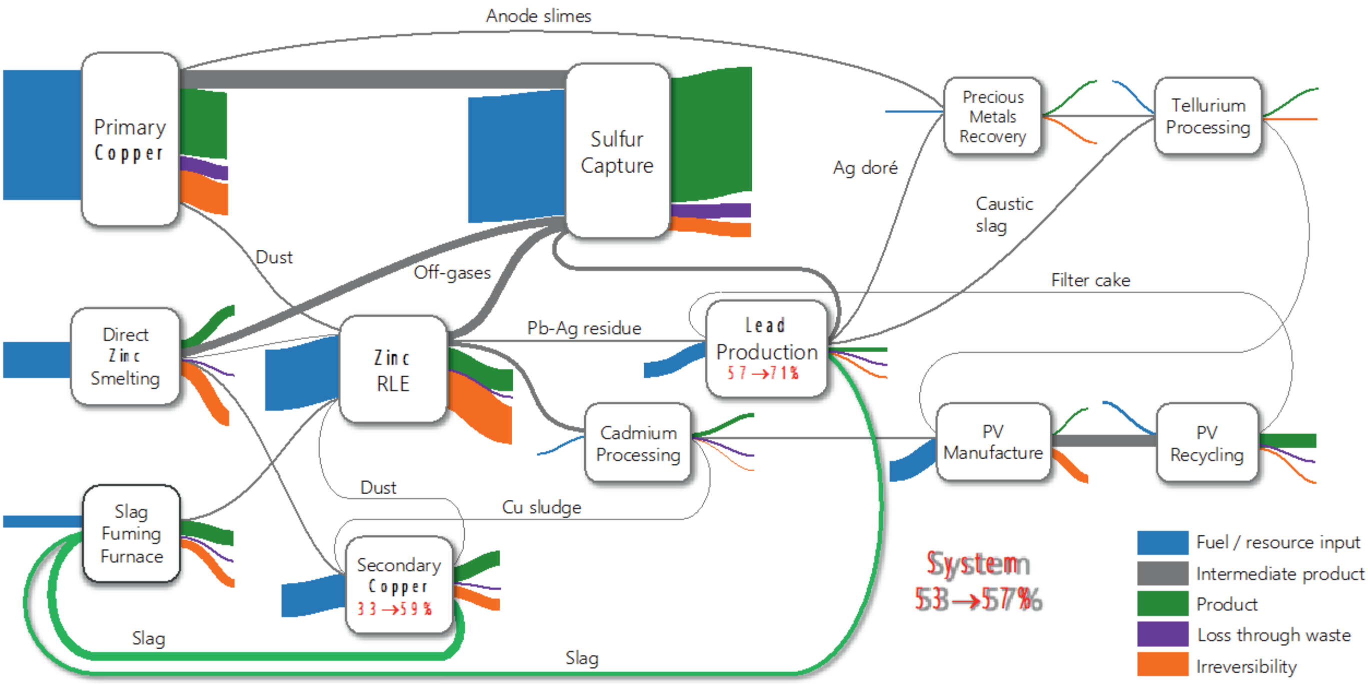


*Figure 5: A Sankey diagram of the exergy flow of the system produced from the HSC Sim simulation model depicted by Figure 4 – showing how the exergy efficiency is improved from 53 to 57 % by recycling the slags from lead and copper production as shown (Bartie et al. 2020).*

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- Comparison of different processing routes for residues from metallurgical processing linked also to cement production (Abadías et al. 2020).

In order to show some detail of the capability of the simulation platform the manufacture of CdTe photovoltaic cells is shown (Bartie et al. 2020). Figure 3 provides a schematic of the system that links the Cu, Pb and Zn production producing the technology elements that are used for the CdTe production (see the Metal Wheel Figure 2 for details). In Figure 3 each carrier metal production infrastructure and materials are represented by Figure 1 linking all the energy requirements of the system completely. This is what has to be mapped simultaneously to understand fully the flow of energy as power and materials as well as the exergy dissipation from the system.

The large number of reactors, flows and compounds have to be mapped to quantify the performance of the circular economy of CdTe-PV systems. This detail is best captured by a simulation tool as depicted by Figure 4.

Using the simulation tool, a basis is created to evaluate the performance of the system. This included the environmental impact using the HSC Sim LCA and thermoeconomic tools (Figure 5). In addition, detail economic analysis of the system can be made based on the results of the rigorous simulation model of the CE system. While the exergy dissipation is shown by Figure 5, detailed environmental impact assessment can be consulted in Bartie et al. (2020).

## Quo Vadis?

We believe the only manner to fully understand the circular economy is by the use of rigorous simulation models. It is clearly shown that this can be done and should in future be the underlying method to quantify the economic, technological as well as the environmental performance of the CE system. Linking to the United Nations Sustainability Developments Goals (SDGs) is of great importance and should be based on the simulation tools briefly presented here and also discussed more comprehensively by Reuter et al. (2016).

While it is tempting to use black box methods such as used in artificial intelligence (AI) to try to optimize and understand such CE systems, it is not recommended. Reuter et al. (1993) showed that it is best to link fundamental approaches with data-AI-driven methods applying hybrid approaches (a mix of methods) to always ensure that the physics is represented in the data that describes and calibrates the models. If the data is of poor quality and methods are used that have no physics laws embedded in them (such as material flow analysis) this will lead to erroneous results.

The path ahead must include the representation of large CE systems as digital twins on the basis of rigorous process simulation. It is a daunting task to create the large models, however, it must be done to fully understand the losses from the system, especially the exergy, as these ultimately affect the economic viability of the CE system. All of the rigorous results provided by the digital twin to the SDGs have to be linked in a suitable manner and made widely accessible to as many stakeholders as possible. Multi-criteria optimization will be indispensable to search for optimal solutions in a very complex parameter space using the results produced by the digital twin, achieved through a surrogate function that can be explored to find the optimum resource efficiency of the system as a function of the numerous influencing independent system parameters.

## References


Abadías Llamas, A., Valero Delgado, A., Valero Capilla, A., Torres Cuadra, C., Hultgren, M., Peltomäki, M., Roine, A., Stelter, M., Reuter, M.A. (2019): Simulation-based exergy, thermo-economic and environmental footprint analysis of primary copper production. Minerals Engineering, 131, 51-65.

Abadías Llamas, A., Bartie, N., Heibeck, M., Stelter, M., Reuter, M.A. (2020). Simulation-based exergy analysis of large circular economy systems: Zinc production coupled to CdTe photovoltaic module life cycle. Journal of Sustainable Metallurgy, 6(1), 34-67.

Apple (2017) http://www.theweek.co.uk/apple/83829/apple-to-make-all-its-products-from-recycled-materials

Bartie, N., Abadías Llamas, A., Heibeck, M., Fröhling, M. Volkova, O., Reuter, M.A. (2020). The simulation-based analysis of the resource efficiency of the circular economy – the enabling role of metallurgical infrastructure. Mineral Processing and Extractive Metallurgy (TIMM C) 129, 2, 229-249.

Beaulieu, Luce; van Durme, Gabrielle; Arpin, Marie-Luc (2016): Circular economy. A critical literature review of concepts. Montréal, Québec, Ottawa, Ontario: CIRAIG; Canadian Electronic Library.

Blanpain, Reuter, Malfliet (2019): Lead Policy Brief: https://www.linkedin.com/feed/update/urn:li:activity:6531862315858423808

Blomsma, F.; Brennan, G. (2017): The Emergence of Circular Economy. A New Framing Around Prolonging Resource Productivity. Journal of Industrial Ecology, 21(3), 603-614.

Bocken, N.M.P., Olivetti, E.A., Cullen, J.M., Potting, J. and Lifset, R. (2017) Taking the Circularity to the Next Level – A Special Issue on the Circular Economy, Journal of Industrial Ecology, 21(3), 476-482.

Ciacci, L., Reck, B.K., Nassar, N.T. and Graedel, T.E. (2015) Lost by Design, Environ. Sci. Technol., 49, 9443–9451.

Ellen Macarthur Foundation "Circular Economy" https://www.ellenmacarthurfoundation.org

EU (2015) Closing the loop – An EU action plan for the Circular Economy https://ec.europa.eu/growth/industry/sustainability/circular-economy_en

EU (2020) Circular Economy Action Plan For a cleaner and more competitive Europe https://ec.europa.eu/environment/circular-economy/pdf/new_circular_economy_action_plan.pdf

Fairphone: Ballester, M., van Schaik, A. and Reuter, M.A. (2017) Fairphone's Report on Recyclability-Does modularity contribute to better recovery of materials? https://www.fairphone.com/en/2017/02/27/recyclable-fairphone-2/ and https://www.fairphone.com/en/2017/08/08/examining-the-environmental-footprint-of-electronics-recycling/

Fernandes, I.B., Abadías Llamas, A., Reuter, M.A. (2020): A simulation-based exergetic analysis of NdFeB permanent magnet production to understand large systems, Journal of Metals (online).

GaBi 8 Thinkstep (2018) https://www.thinkstep.com

Ghisellini, P.; Cialani, C.; Ulgiati, S. (2016): A review on circular economy. The expected transition to a balanced interplay of environmental and economic systems. Journal of Cleaner Production, 114, 11-32.

Jackson, M.; Lederwasch, A.; Giurco, D. (2014): Transitions in Theory and Practice. Managing Metals in the Circular Economy. Resources, 3(3), 516-543.

Kirchherr, J., Reike, D., Hekkert, M. (2017): Conceptualizing the circular economy. An analysis of 114 definitions. Resources, Conservation and Recycling 127, 221-232.

Lansink, A. (2017): Challenging Changes. Connecting Waste Hierarchy and Circular Economy. ISBN/EAN 978-90-821783-5-7. NUR973. 398p.

Lieder, M., Rashid, A. (2016): Towards circular economy implementation. A comprehensive review in context of manufacturing industry. Journal of Cleaner Production, 115, 36-51.

Mendoza, J.M.F., Sharmina, M., Gallego-Schmid, A., Heyes, G. and Azapagic, A. (2017) Integrating Backcasting and Eco-Design for the Circular Economy, Journal of Industrial Ecology, 21(3), 526-544

Homrich, A.S.; Galvão, G.; Abadia, L.G.; Carvalho, M.M. (2018): The circular economy umbrella. Trends and gaps on integrating pathways. Journal of Cleaner Production, 175, 525-543.

Outotec (2020) HSC Chemistry 10 Outotec http://www.outotec.com/products/digital-solutions/hsc-chemistry

Reuter, M.A., Van der Walt, T., Van Deventer, J.S.J. (1993): A generalized neural net kinetic rate equation. Chemical Engineering Science, 48(7), 1281-1297.

M.A. Reuter (1998): The simulation of industrial ecosystems. Minerals Engineering, 11(10), 891-917.

Reuter, M.A. and Van Schaik, A. (2012) Opportunities and limits of recycling: A dynamic-model-based analysis, MRS BULLETIN, 37(4), 339-347.

Reuter, M.A. and Van Schaik, A. (2015) Product-centric simulation-based design for recycling: greenprinting of LED lamp recycling, Journal of Sustainable Metallurgy, 1(1), 4-28.

Reuter, M.A., Van Schaik, A. and Gediga, J. (2015) Simulation-based design for resource efficiency of metal production and recycling systems: Cases-copper production and recycling, e-waste (LED lamps) and nickel pig iron, The International Journal of Life Cycle Assessment, 20(5), 671-693.

Reuter, M.A. (2016) Digitalizing the Circular Economy-Circular Economy Engineering defined by the metallurgical Internet of Things-, 2016 TMS EPD Distinguished Lecture, USA, Metallurgical Transactions B, 47(6), 3194-3220 https://link.springer.com/article/10.1007/s11663-016-0735-5

Reuter, M.A. Van Schaik, A., Ballester, M. (2018): Limits of the Circular Economy: Fairphone Modular Design Pushing the Limits, World of Metallurgy – Erzmetall 71(2), 68-79.

Reuter, M.A., Van Schaik, A., Gutzmer, J., Bartie, N., Abadías Llamas, A. (2019): Challenges of the Circular Economy – A material, metallurgical and product design perspective. Annual Review of Materials Research, 49, 253-274.

Reuter (2019): Design for Recycling – Inconvenient truths of the circular economy https://annualreport2018-19.aurubis.com/magazine/rethink/design-for-recycling

Schaik, A. van and Reuter, M.A. (2016) Recycling indices visualizing the performance of the circular economy, World of Metallurgy – ERZMETALL, 69(4), 201-216.

UNEP – United Nations Environment Programme. International Resource Panel, issuing body (2013): M.A. Reuter, C. Hudson, A. van Schaik, K. Heiskanen, C. Meskers, C. Hagelüken, Metal recycling. Opportunities, limits, infrastructure / International Resource Panel. Nairobi: UNEP. http://www.resourcepanel.org/reports/metal-recycling

United Nations Sustainability Developments Goals (SDGs) https://sustainabledevelopment.un.org/?menu=1300

Verhoef, E., Dijkema, G. and Reuter, M.A. (2004) Process knowledge, system dynamics and metal ecology, Journal of Industrial Ecology, 8(1-2), 23-43.