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Case studies for aluminium

Doctoral thesis

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Il faut absolument que les hommes parviennent à préserver autre chose que ce qui leur sert à faire des semelles, ou des machines à coudre, qu'ils laissent de la marge, une réserve, ou il leur serait possible de se réfugier de temps en temps. C'est alors seulement que l'on pourra commencer à parler d'une civilisation[1].

— Romain Gary, *Les Racines du ciel, 1956.*

[1] It's absolutely essential that man should manage to preserve something other than what helps to make soles for shoes or sewing machines, that he should leave a margin, a sanctuary, where some of life's beauty can take refuge and where he himself can feel safe from his own cleverness and folly. Only then will it be possible to begin talking of civilization.

— Romain Gary, *The Roots of Heaven*, 1956 (translated by Jonathan Griffin).

PREFACE

This thesis has been submitted to the Faculty of Engineering Science and Technology (IVT) in partial fulfilment of the requirements for the degree of Philosophiæ Doctor. This work was carried out at the Industrial Ecology Programme (IndEcol) and the department of Energy and Process Engineering (EPT) at the Norwegian University of Science and Technology (NTNU) in Trondheim, Norway, in the period 2017-2022, under the supervision of Prof. Daniel Beat Müller and the co-supervision of Prof. Jonathan Cullen.

This research was funded by the Centre for Research-Based Innovation, SFI Metal Production, (NFR Project n°237738), and by the Norwegian Research Council (BATMAN Project, NFR Project n°299334).

ABSTRACT

Metal cycles form the backbone of our modern societies but are also responsible for a large part of the anthropogenic greenhouse gas (GHG) emissions. The transition towards a more sustainable socio-economic metabolism will require large quantities of metals. Aluminium, thanks to its use in transport, buildings, electronics and energy systems, is a key element to realise this transformation. This thesis is proposing the use of new tools for monitoring and simulating the future of metal cycles and their emissions at different scales, using the aluminium cycle as the main example for applications.

The approach developed for monitoring material cycles and is based on two main components: (1) a framework for designing maps of the physical economy at the societal scale, with the aim to better inform sustainability strategies, and (2) a physical accounting framework to monitor material use and emissions of industrial plants based on the application of multilayer material flow analysis at the plant-level.

The dynamic MFA tools developed in this thesis increase the granularity of models used for the simulation of metal cycles. The four major methodological contributions are (1) a general framework and classification for models studying the dynamics of stocks within systems, which enables the creation of a common language to foster the cross-field dissemination of models; (2) a framework for modelling the stock dynamics of product-component systems to allow modelers to better study circular economy strategies, such as reuse and replacement; (3) a combined lifetime-leaching approach that enables the simulation of radical transformation strategies, such as the early demolition of old buildings to accelerate the penetration of energy-efficient ones; (4) a new scenario-rich approach based on multilayer MFA that allows modellers to better capture the transformation of products and technologies over time and to analyse how these changes in characteristics influence primary material demand and the potential for recycling.

These tools where applied to different case studies: the monitoring of emissions in an aluminium smelter, scenarios for the future demand of materials for lithium-ion

batteries, scenarios for the future demand of aluminium in cars, and scenarios for the future energy use and emissions for the Swiss building stock.

Our main results show that the demand for aluminium and other battery materials in transport applications will considerably increase within the next decades. For aluminium, the changes in alloy requirements driven by electrification make the occurrence of a significant scrap surplus very likely, which would severely limit the contribution of recycling to climate change mitigation in the absence of alloy-sorting technologies or increased dismantling of car components. Even if options to decarbonise primary production exist, both for direct emissions at plant-level and for the electricity supply, most of them would take time to implement and a rapid surge in primary aluminium demand will a result in a large increase of GHG emissions. To reduce emissions from metal production during this transition phase, a comprehensive approach is necessary. Policies and measures that would only target the carbon footprint of cars and batteries do not consider systemic effects, such as the recycling challenges created by the possible occurrence of a scrap surplus in the future. They might also result in burden shifting to other sectors, which does not help in reducing the overall GHG emissions. Solving these issues and optimising the whole system would require better coordination between the different actors in the supply chain, both in primary and secondary production, product manufacturing and end-of-life management. Robust monitoring tools and large-scale simulation models can facilitate this cooperation and help decision makers quantify and target the investments needed for decarbonising material cycles.

Acknowledgements

First of all, I would like to thank my supervisor Daniel Müller for his excellent guidance, support, and patience during those five years. From the first MFA lectures in 2010, to the master thesis and all along this PhD, he has been a constant source of inspiration. I learned a lot from him, both as a scientific role model, who values integrity and passion for good research above all, but also as a great person who always put people first and is always there to listen and help when needed.

I express my gratitude for the many insights and advice I got from people I met working on different projects: the members of the SFI Metal Production who introduced me to the secrets of metallurgy, especially Casper Van der Eijk, Leiv Kolbeinsen, Anne Kvithyld and Gabriella Tranell, the partners of the BATMAN project, Stina Torjesen, Lars Petter Maltby, Christian Rosenkilde, and all the workshops participants, and the great people I met during the MinFuture project, especially Maren Lundhaug for her help at the start of my PhD, Evi Petavratzi for her insights from the mineral world, and Jonathan Cullen who kindly accepted to become my co-supervisor.

I would also like to thank all my co-authors, especially Felipe and Dirk for the many stock dynamic meetings that were successful at last, Marta for great discussions and GitHub interactions, Even and Morten who made all the projects with Hydro possible, and Louis who did an incredible job at deciphering all the plant data. Special thanks are due to Fernando, my best battery friend and eternal partner in fighting modelling crime.

Thank you also to all fellow PhD students, old and new Indecol colleagues and friends, for a wonderful "work" atmosphere. I am particularly grateful to the MFA group, my office mates Carine, Sahin, Homa, Daniel, and Nils, the sunny office people Miguel, Johana, Marthe, Kajwan, Lorenzo, Cristina, Thomas, and Baptiste, who are always there when you do not need a coffee break, and Alex, Martin, Koen, Dan, John, Max, Jia-Jia, Kamila, Lola, Avi, Meng, and all the Jans. I cannot name everyone here but I could never have stayed that long without all of you!

I would also like to thank the IndEcol students I met in classrooms or cabins over the years for breaking the monotony of research, especially those I co-supervised for their master project or thesis: Louis (who helped turning his excellent thesis in a paper), Valentin, Thomas, Giulia, Håvard, Sofia, Eric, Brent, Marceau, and Moritz. This thesis would have been much harder to write without your help.

Thanks also to all the gliding, rugby, climbing, skiing, sailing and chilling friends that make living in Trondheim a special experience.

My final thanks go to my family, my parents who always encouraged my curiosity and let me find my own way, and Marion who really made this thesis possible by coming all the way to Trondheim and supporting me (both according to the French and English definitions) during those five years, despite all the grumpiness, bad weather, and disputable food quality.

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List of Appended Publications and Author's Contribution

	Title and authors	Author's contribution
1	*Maps of the physical economy to inform sustainability strategies* Müller, D.B.; Billy, R.G.; Simoni, M.U; Petavratzi, E.; Liu, G.; Rechberger, H.; Lundhaug, M.C. & Cullen, J. in *Handbook of Recycling 2nd ed., Ch. 4, Elsevier* *(accepted for publication)*	Concept development for chapters 4-5 and writing.
2	*Systemic Approaches for Emission Reduction in Industrial Plants Based on Physical Accounting: Example for an Aluminum Smelter* Billy, R.G.; Monnier,L.; Nybakke, E.; Isaksen, M. & Müller, D.B. *Environ. Sci. Technol.* 2022 *56* (3), 1973-1982 DOI: 10.1021/acs.est.1c05681	Research design, data collection, modelling, analysis, visualisations, and writing.
3	*A general framework for stock dynamics of populations and built and natural environments* Lauinger, D.; Billy, R.G.; Vásquez, F. & Müller, D.B. *J Ind Ecol*. 2021; 25: 1136-1146. DOI: 10.1111/jiec.13117	Research design, literature review, framework development, and writing.
4	*A product-component framework for modelling stock dynamics and its application for electric vehicles and lithium-ion batteries* Aguilar Lopez, F.; Billy, R.G. & Müller, D.B. *J Ind Ecol*. 2022 (published online) DOI: 10.1111/jiec.13316	Research design, framework development, modelling, analysis, and writing.
5	*Evaluating strategies for managing resource use in lithium-ion batteries for electric vehicles using the global MATILDA model* Aguilar Lopez, F.; Billy, R.G. & Müller, D.B. (under review, *Resources, Conservation & Recycling*)	Research design, support for the modelling task, analysis, and writing.
6	*Aluminium use in passenger cars poses systemic challenges for recycling and GHG emissions* Billy, R.G. & Müller, D.B. (under review, *Resources, Conservation & Recycling*)	Research design, data collection, modelling, analysis, visualisations, and writing.

7	*Pathways toward a carbon-neutral Swiss residential building stock* Roca-Puigròs, M., Billy, R.G., Gerber, A., Wäger, P. and Müller, D.B., 2020. *Buildings and Cities*, 1(1), pp.579–593. DOI: 10.5334/bc.61	Research design, support for the modelling task, analysis, and writing.

1 INTRODUCTION

1.1 CONTEXT AND MOTIVATION

The overall objective of this project is to improve the understanding of the relationships between metal cycles and the society, using aluminium as a case study. This work is proposing new methodologies within Material Flow Analysis (MFA) to monitor and simulate the future evolution of metal cycles and their associated emissions, at different scales. The case studies refine the understanding of the global aluminium cycle and its likely evolution, via an extended scenario analysis.

1.2 SOCIO-ECONOMIC METABOLISM AS A FRAMEWORK TO STUDY SUSTAINABILITY

Humanity has been able to thrive and develop on Earth for thousands of years, without fear of running out of the essential resources or of threatening Earth's life support systems. However, the increase in population and affluence level made possible by progress in science and technology now raise the issue of the maximum carrying capacity of the Earth system, questioning economic growth, its characteristics (Arrow et al. 2009) and the way to measure wealth (Dasgupta 2010).

For more than two centuries, the scientific community has been aware of the existence of natural limits to exponential growth (Malthus 1798; Verhulst 1838). Indeed, climate change, environmental pollution, resource depletion, and changing demographics are some of the most pressing problems of our time. The impacts of our industrialized societies on nature and our own living environment can no longer be ignored, as anthropogenic cycles now dominate natural cycles for most chemical elements (Klee and Graedel 2004). This has even led to the proposition of Anthropocene as a new geological epoch (Crutzen and Stoermer 2000; Steffen et al. 2011). More recently, Rockström et al. (2009) have defined planetary boundaries for nine types of environmental impact categories, defining a safe operating space for humanity, which is likely to be reduced if we miss the institutions and knowledge required to avoid the depletion of our common resources (Hardin 1968). The question is no more on the existence of these limits, but rather on how to ensure continuous human development under physical constraints. This involves realizing a shift between socio-economic regimes (Fischer-Kowalski 2011), towards a so-called "spaceman economy" (Boulding 1966).

When exploring potential *Limits to Growth* using System Dynamics, Meadows et al. (1972) illustrated how the study of interactions between different system components can provide important insights, and shed light on complex feedback mechanisms that would otherwise be missed without a holistic approach.

The linkages between different components of sustainability (Graedel and Van der Voet 2009), as well as the complex relationships between natural and anthropogenic environments and within them need to be studied using a systemic framework, such as the industrial metabolism (Ayres 1989), the anthropogenic metabolism (Baccini and Brunner 1991), and later the socio-economic metabolism (SEM) (Fischer-Kowalski 1998; Pauliuk and Hertwich 2015).

1.3 The role of natural and geological stocks for the study of the socio-economic metabolism

The SEM can only function thanks to the "free" ecosystem services enjoyed from nature. Costanza et al (1997) evaluated their economic value to be in the range of 16 to 54 trillion $ per year, which was in the range of the global GDP at that time. They also pointed out the fact that these services depend on the natural capital stocks that produce them.

Later, this notion of natural capital stocks was expanded as Costanza et al. (2007) demonstrated that the quality of human lives depends on the "opportunities that are provided to meet human needs in the forms of built, human, social and natural capital (in addition to time) and the policy options that are available to enhance these opportunities". Discussed in light of resource scarcity, this statement implies that a sustainable society must find a balance between its use of resources (increasing scarcity) and the speed at which its technology develops (effectively decreasing scarcity by finding new resources and improving existing processes). Failing to do so will result in an "ingenuity gap", where societies cannot find in time the intellectual resources to adapt to increased scarcity (Homer-Dixon 1995).

Furthermore, not understanding correctly the dynamic behaviour of some resources or natural cycles can lead to faster depletion and stronger environmental impacts (Moxnes 2000). For minerals, using static depletion rate models usually leads to an overestimation of the scarcity, especially if it is combined with the common assumption of using currently known resources or reserves (which depend on economic and technological conditions at a given time) as a proxy for the total available resources. For instance, (Frosch and Gallopoulos 1989) calculated the estimated time to depletion for some major global resources, using estimates for resources and reserves from 1989 and consumption rates from 1989 and 2030. They derived estimates as low as 3 years for petroleum reserves with 2030 consumption rates. Even if it can be used to compare the relative scarcity of different resources under current conditions, this type of approach is not relevant for prospective analysis and leads to many shortcomings. The dynamic character of reserves and resources (determined by geology, but also by technological and economic conditions) and our use of them need to be taken into account, as well as the evolution of anthropogenic cycles.

Dynamic models that evaluate the available resources both in a geological and techno-economic perspective have been developed for example for copper, for which resource depletion is a major issue (Gordon et al. 2006; Sverdrup et al. 2014; Northey et al. 2014; Singer 2017). However, these system dynamics and economic models lack a strong system definition of the anthropogenic cycle of the metal, as in a Material Flow Analysis (MFA), a method commonly used to study and quantify the SEM. An MFA is a systematic assessment of the flows and stocks of materials within a system defined in space and time (Brunner and Rechberger 2016). This distinction is even more important for aluminium, for which resource depletion in itself is not a main concern (Graedel 2011) compared to the energy use and the environmental impacts of primary production.

1.4 THE ROLE OF ANTHROPOGENIC STOCKS FOR THE STUDY OF THE SOCIO-ECONOMIC METABOLISM

The idea to use anthropogenic stocks as a driver for the study of the SEM is not new. More than twenty years ago, Baccini and Bader (1996), then Van der Voet et al. (2002) proposed to use the characteristics of stocks to predict future emissions. Indeed, according to Pauliuk and Müller (2014), human well-being can be linked to the level of services enjoyed from the physical environment, which is better quantified in a long-term perspective by the level of in-use stocks in the socio economic metabolism. These anthropogenic in-use stocks are key to study environmental impacts from human activities and to design long-term climate mitigation strategies, for three main reasons: (1) "in-use stocks link the services enjoyed by humans to energy and material consumption" (Pauliuk and Müller 2014); (2) the building of these stocks is in itself one of the largest driver for energy and material use, and hence crucial for the study of decoupling strategies; (3) the long-term nature of stocks in the built environment and associated lock-in effects define an envelope for possible or impossible trajectories for future emissions. To illustrate these points, Müller et al. (2013) calculated that under current technologies, carbon emissions from the production of new materials related to infrastructure development would represent 35 to 60 % of the total available carbon budget if developing economies would reach the same in-use stocks level as Western countries. Similarly, Krausmann et al. (2017) calculated that global material stocks rose 23-fold over the 20th century and that their maintenance requires half of the current annual resource use. They also concluded that a convergence of the global per-capita stocks to the level of Western economies will lead to an increase of stocks by a factor 4, which is not compatible with climate mitigation targets.

1.5 THE IMPORTANCE OF METAL CYCLES AND ALUMINIUM FOR SUSTAINABILITY

Material production is currently responsible for more than 50 % of industrial greenhouse gas (GHG) emissions, dominated by steel, cement, plastic, paper and aluminium (Allwood, Cullen, and Milford 2010). Steinberger et al. (2010) concluded that "Human use of materials is a major driver of global environmental change", while showing a strong income elasticity and large inequalities across countries and socio-economic groups. They also established that this inequality is the most striking for ores and industrial minerals, which are the material group whose consumption exhibits the highest Gini coefficient between rich and poor populations. Understanding patterns of material use is therefore paramount for designing decoupling strategies for a sustainable future in which human needs can be satisfied without jeopardizing the natural environment (Steinberger and Roberts 2010).

Metal cycles in particular are important for the study of the SEM and climate change mitigation. Because of the chemical properties of metallic elements, metal production is highly energy intensive, while recycling usually requires only a fraction of the energy needed for primary production. For this reason, thanks to their variety of interesting properties and recycling potential, metals can be considered as a basis for a sustainable society, at the condition to design closed recycling loops with limited loss of quality and impacts on the environment (von Gleich 2006).

Aluminium is an extreme example: secondary production requires only from 5 to 10 % of the energy use of primary production (Quinkertz, Rombach, and Liebig 2001). Despite being the most abundant metal on Earth, it has only been commercially produced after the invention of the Hall-Héroult and Bayer processes, respectively in 1886 and 1888, and only became a major industrial metal in the 20th century, during which it experienced an exponential growth. This relatively recent use compared to iron or other major metals, combined with its durability and ease of recycling, is the reason why 75% of all aluminium ever produced is believed to be still in productive use today (Marlen Bertram, Martchek, and Rombach 2009; M. Bertram et al. 2017).

One of the most recent quantifications of the impacts of the global flow of aluminium show that aluminium production is responsible for 3.5% of the global electricity use and 1% of global CO2 emissions (Cullen and Allwood 2013). This appears small compared to the impacts of steel or concrete production, but contrarily to iron, even the most advanced countries currently show no signs of saturation for the level of per-capita in-use aluminium stocks (Liu and Müller 2013).

Hence, the International Energy Agency forecasts that the global demand for aluminium will rise from 80 Mt/yr in 2017 (IAI, International Aluminium Institute 2019) to between 110 and 153 Mt/yr in 2050 (IEA 2009). While the energy intensity of aluminium primary production declined by 1.1% in in 2017 compared to 2016, the global primary production increased by 5.9%, resulting in a 5% increase in energy demand (IAI, International Aluminium Institute 2019). In accordance with these trends, Liu et al. (2013) have forecasted that the climate target of reducing GHG emissions by 2050 to 50% of 2000 levels is only reachable for the aluminium industry if per capita stocks converge rapidly to a low saturation level, even under the most techno-optimist scenarios. This conclusion shows that to decarbonize the aluminium industry, it is necessary to combine demand reduction, radical new technologies in primary production, and increased post-consumer scrap recycling.

The challenge ahead seems even greater as the exponential growth of aluminium use has had a record of repeatedly outgrow similar predictions about future aluminium demand. For instance, Kuckshinrichs and Poganietz (2006) used the partial-equilibrium model GlobAl from Schwarz et al. (2000) to predict a maximum global primary aluminium production of 31 Mt in 2010 (this was the highest of three scenarios, the lowest being 25 Mt). In reality, the world produced 42,3 Mt of primary aluminium in 2010 (International Aluminium Institute 2022), despite the effects of the global economic crisis that was not anticipated in the scenario analysis. Even if the models have been greatly improved since, notably thanks to the use of dynamic material flow analysis and trade data, this retrospective analysis illustrates the fact that even the most pessimistic (in climate terms) scenarios can largely underestimate the growth rates of the aluminium industry and the associated environmental impacts.

1.6 Monitoring of metal cycles and their emissions

It is therefore crucial to monitor the evolution of metal cycles and their emissions. Detailed maps of the physical economy would enable a better understanding of the SEM and the potential for improving its sustainability. However, current data collection and monitoring frameworks are fragmented, lack a systemic approach, and do not respect mass and energy balance principles. Approaches based on Life Cycle Assessment (LCA) suffer from several weaknesses, such as the lack of clear geographical and temporal boundaries and the limitations inherent to the allocation approach used for recycling and GHG emissions (Liu and Müller 2012). These limitations make it hard to consider issues that are relevant for the overall metal cycles, such as the pressure on natural resources or the challenges for recycling created by the characteristics of new products. There is thus a need for approaches that can be more robustly scaled up from a single plant or the production of a single product to the wider metal cycle.

Carbon reporting frameworks and emission trading schemes (ETS) currently used to report GHG emissions and trade quotas between companies also suffer from methodological limitations. Results are highly aggregated at the level of industrial installations, which are only required to report their total emissions. Differences in scope and in the application of the accounting methodologies also make it hard to draw meaningful comparisons between different sites (Bellassen et al. 2015). Finally, incomplete coverage and the lack of incentive for circular economy strategies such as reuse or recycling limit the implementation of material efficiency measures. At the same time, approaches that are robust at process level, such as flowsheeting, are usually missing a connection to the wider context of the plant and its linkages with the outside world. They also lack the temporal component needed to consider the influence of the changes in inventories of raw materials and products over time. As such, they are not able to assess the real potential of systemic mitigation strategies, even when they include a connection between material use and GHG emissions (Porzio et al. 2013).

Another issue arising from unsatisfactory reporting methodology is that the resulting data is too inconsistent to be scaled up and uncover and evaluate systemic options for resource use and emissions reduction at a larger scale. Statistics based on poor or incomplete data from reporting tools that lack a system definition might lead to a misinterpretation of data points, and a generalisation of incomplete measurements without proper consideration of the associated uncertainties. This is problematic for the collection and aggregation of industry data to generate the national and international statistics needed to draw the robust maps of the physical economy upon which modelers can build simulation models to inform future strategies.

To try to overcome these limitations and understand the impacts associated with the production of aluminium along its value chain, several quasi-stationary MFA models have been developed the last 20 years. These models usually only consider flows and stocks accumulation in a given year, without taking into account longer-term dynamic effects influencing the development of stocks and scrap availability. Here are some examples of quasi-stationary MFA models studying aluminium, classified according to their scope in term of geographical or products coverage:

- Regional level: Europe (Passarini et al. 2018; Boin and Bertram 2005)
- Country level: USA (Plunkert 2006; Liu, Bangs, and Müller 2011; W.-Q. Chen et al. 2016), Denmark (Hansen and Lassen 2003), Italy (Amicarelli, Lagioia, and de Marco 2004; Ciacci et al. 2013), China (W. Chen, Shi, and Qian 2010; W. Q. Chen and Shi 2012)
- Product or alloy specific: beverage cans (Løvik and Müller 2014; Buffington and Peterson 2013), extruded alloys used in building applications in France (Billy 2012), automotive alloys (Peterson 2015).

However, little research has been conducted at smaller scales, and if plant-level MFA studies have existed since the first years of existence of the field (Belevi and Moench 2000), they have remained much more seldom. More recently, some plant-level studies have been conducted for the steelmaking industry (Gonzalez Hernandez et al. 2018), but none for aluminium, despite being one of the most analysed metal in MFA studies. The strength of MFA compared to other monitoring tools is its capacity to consistently link over time energy use and emissions with material stocks and flows in a system context. Increasing the granularity of models by looking more specifically at individual plants could generate insights that would greatly improve the capabilities of MFA as a reporting tool and enable better bottom-up monitoring of material cycles. Different plants have different emission performance and analysing them in more details would enable to go beyond the industry averages that are used in larger scales models.

1.7 Scenario analyses for the future evolution of metal cycles

Dynamic models have first been used as simulation tools for the future evolution of metal cycles in the 1970s to quantify the future availability of stocks and flows of secondary aluminium, and hence the potential for recycling. The first models were econometric or partial-equilibrium models, which can be considered as flow-based models (Fisher, Cootner, and Baily 1972) for copper, (Bever 1976; Hojman 1981; Brown et al. 1983; Blomberg and Hellmer 2000; Schwarz, Kruger, and Kuckshinrichs 2000) for aluminium. This approach has been refined and updated since (Liu and Müller 2013; Maung et al. 2017), and used at country-level: Germany (Melo 1999), Austria (Buchner et al. 2017), the U.S. (McMillan et al. 2010; Hatayama et al. 2007). Strictly speaking, dynamic MFA has first been applied to aluminium in the United States (Liu, Bangs, and Müller 2011; W. Q. Chen and Graedel 2012), then on the global level (Liu, Bangs, and Müller 2013; M. Bertram et al. 2017). Recent studies have been linking scenarios for future metal production with Shared Socioeconomic Pathways (SSPs) (Yokoi, Watari, and Motoshita 2022; Pedneault et al. 2021) and have aimed at identifying a link between the amount of metal use in society (in terms of stock of metal/capita) and climate targets (Watari, Nansai, and Nakajima 2021).

To develop this approach further, and to consider more complex issues related to the scrap quality, demand, and availability, it is necessary to increase the granularity of the models, including more details about the properties of materials, products, and technologies used in the different stages of the value chain. For instance, increasing recycling can lead to impurity accumulation, which is problematic considering the quality requirements for the different aluminium alloys (Løvik and Müller 2014; Peterson 2015). In addition, it has been shown that current recycling practices in the automotive industry rely mostly on cascading, or downcycling (Løvik, Modaresi, and Müller 2014). Low-alloy scrap from wrought aluminium ends up in high-alloy casting alloys, used mainly for the production of engine blocks. Even if this solution is practical and efficient today, this is likely to become an issue in the future (Modaresi and Müller 2012). Indeed, while the scrap availability is projected to increase as more and more products reach end of life, the demand for low quality secondary aluminium is likely to be lower, due to the lower needs of aluminium castings in engine blocks associated with the development of electric vehicles at the expense of conventional internal combustion engines, which can result in a surplus of casting scrap. This risk of a future scrap surplus has been investigated further for Austria (Buchner et al. 2017) and at the global level: Van den Eynde et al. (2022) predicted a global scrap surplus of 5.4 Mt/yr by 2030 and 8.7 Mt/yr by 2040. However, both these studies used a simplified representation of the transport sector compared to previous works. To be able to address these issues, future scenarios should be based on more detailed models that consider the changing composition of products in use, the technologies used for manufacturing them and their alloys requirements, as well as the improvements needed in sorting and recycling technologies to better recover different types of scrap (Modaresi, Løvik, and Müller 2014).

In-use stocks are by nature a marker of the long-term perspective and a factor of continuity for future scenarios. This robustness and low sensitivity to short-term fluctuations explains their use as drivers in prospective SEM studies. However, as time passes without significant changes in the trajectory for global GHG emissions, sustainability targets become progressively out of reach and climate change mitigation pathways rely more on more on radical measures to remain within 1.5- or 2-degrees global warming scenarios. These measures require deeper and faster transformations of the SEM, that can no longer be modelled by scenarios that assume a continuity with patterns of the past. It is therefore necessary to expand the toolbox for dynamic MFA modelling, with new frameworks that open new possibilities to model radical transformative measures. The scale of the change needed further requires a multidisciplinary approach, to combine advances and methods from different fields relevant to sustainability and the SEM, which describes interactions between human populations and the built and natural environments.

1.8 Objectives and Research Questions

This thesis aims at improving the tools necessary to monitor metal cycles and simulate the transformations of the SEM required to evolve towards a more sustainable society. Examples of the application of these tools are provided with several case studies, most of them focusing on the aluminium cycle.

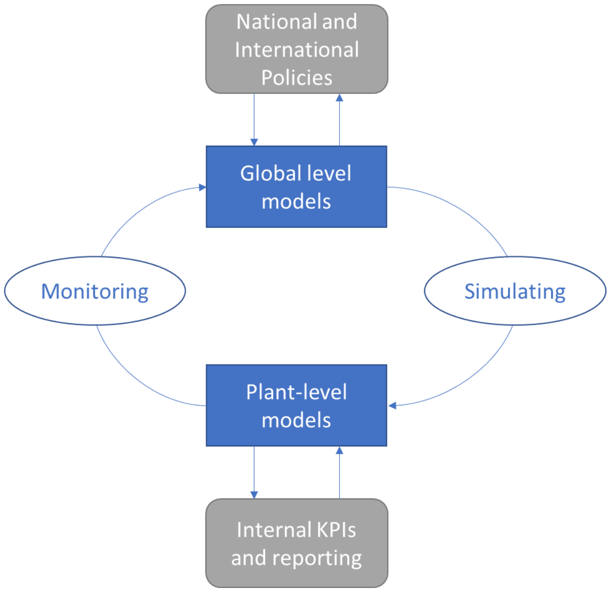

Figure 1: Combining monitoring and simulation models at different scales to generate policy and industry relevant insights

The objectives are to provide answers to the following research questions:

1. **How can metal cycles and their emissions be monitored more effectively based on mass and energy conservation principles?**
   How to design maps of the physical economy based on consistent data? How to reconcile internal reporting and performance indicators with mandatory emission reporting?
2. **How can we facilitate the evaluation of transition strategies for metal cycles using refined simulation models?**

Existing models for simulating the future of metal cycles tend to focus on the global scale and continuity with historic data. What are methodological options to increase the granularity of these models, both in terms of scale, scope, or flexibility to design multiple future scenarios? How can dynamic stock models be extended to reflect the radical systemic changes needed to meet climate targets? How to better model the effects of circular economy strategies, such as reuse and replacements of defect components in products?

3. **How can we apply these monitoring and simulation tools to the global aluminium cycle and its emissions?**

   What are the new insights that can be gained with increasing granularity of these monitoring and simulation tools? The future of the aluminium cycle depends largely on the future demand for aluminium products. This is especially the case for transport applications where aluminium is a material of choice for light-weighting and the transition to electric mobility. What are possible scenarios for future aluminium demand, especially in the fast-growing transport applications? How will they influence the share of primary vs. secondary aluminium production? What are challenges to increase recycling? Which changes in the cycle, in terms of technical innovations, investments, and systemic optimisation are needed to reach climate mitigation targets?

1.9 Structure of the thesis

In **paper 1**, we present the different dimensions of the MFA framework to map the physical economy, with a review of different applications for the aluminium cycle. **Paper 2** introduces the concept of physical accounting based on plant-level multilayer MFA. It is illustrated with an application to an aluminium smelter, in which we apply the physical accounting framework for monitoring GHG emissions and assess the potential of systemic reduction measures. The other chapters focus on improving the modelling toolbox for simulating material cycles. **Paper 3** is presenting a general theory for stock dynamics of populations and built and natural environments, with the aim to provide a common language for the study of stock dynamics in the different fields relevant to sustainability. The basic variables and equations of stock dynamics systems are introduced, and basic models are divided in different classes depending on their fundamental properties. Building on this general theory, **paper 4** is introducing a more advanced framework that enables modelling interactions in systems that are composed of a main product and a component. Thanks to the introduction of hazard functions for the modelling of lifetime and leaching in products and components, the effect of different circular economy strategies can be studied in more detail. 12 elementary cases are presented, together with algorithms to solve the stock dynamics for each of them. The use of the framework is illustrated with a case study on electric vehicles and their lithium-ion batteries, quantifying the effects of different reuse or replacement strategies for reducing future material demand. **Paper 5** applies this framework further to lithium-ion batteries and uses a multilayer dynamic MFA model to consider different scenarios for the future demand of eight battery materials. **Paper 6** is focusing on aluminium and models its future use in passenger cars to quantify the impact that current trends (such as light-weighting, electrification, consumer performance for larger cars, and growing car ownership) have on aluminium demand, recycling limitations due to potential scrap surplus, and the consequences for GHG emissions from aluminium production. Finally, **paper 7** introduces a combined lifetime-leaching approach for stock-driven dynamic MFA models to model the effects of early replacements of stocks (before the end of their theoretical lifetime). This enables studying the effect of more radical scenarios, in which transformations are accelerated by forced removing of old cohorts from the stock. The use of the method is illustrated by the effect of early replacements on future energy demand and emissions from Swiss buildings.

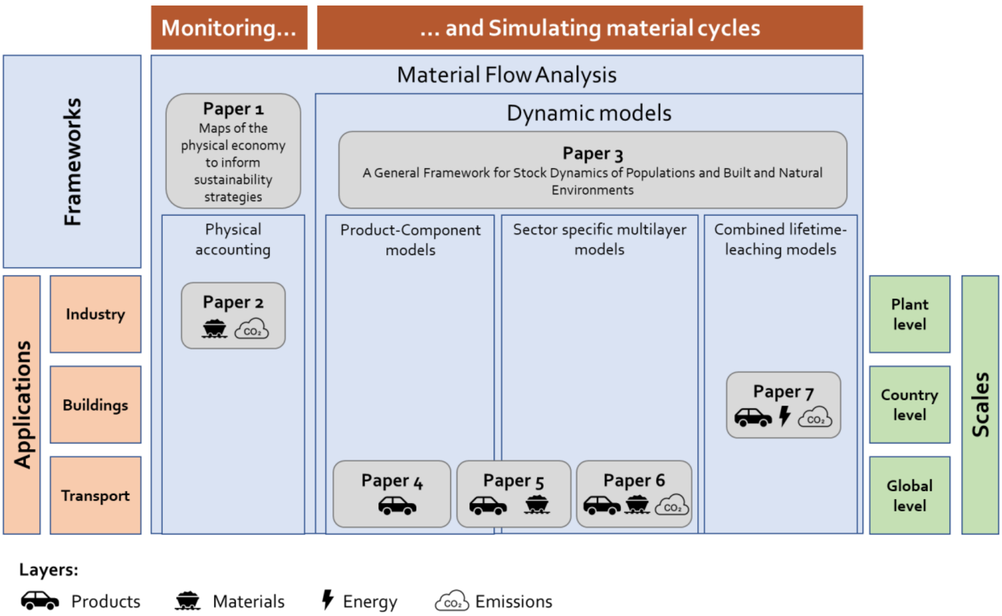

Figure 2: Graphical structure of the thesis and overview of the appended papers

2 METHODS

2.1 MATERIAL FLOW ANALYSIS AS A TOOL TO MONITOR THE PHYSICAL ECONOMY

The work presented in this thesis builds upon Material Flow Analysis (MFA) or Substance Flow Analysis (SFA), as defined by Baccini and Brunner (1991) and Baccini and Bader (1996). This definition is expanded in paper 1, which states that a main characteristic of MFAs is that they explicitly cover the four dimensions of stages, trade, layers, and time (Figure 3).

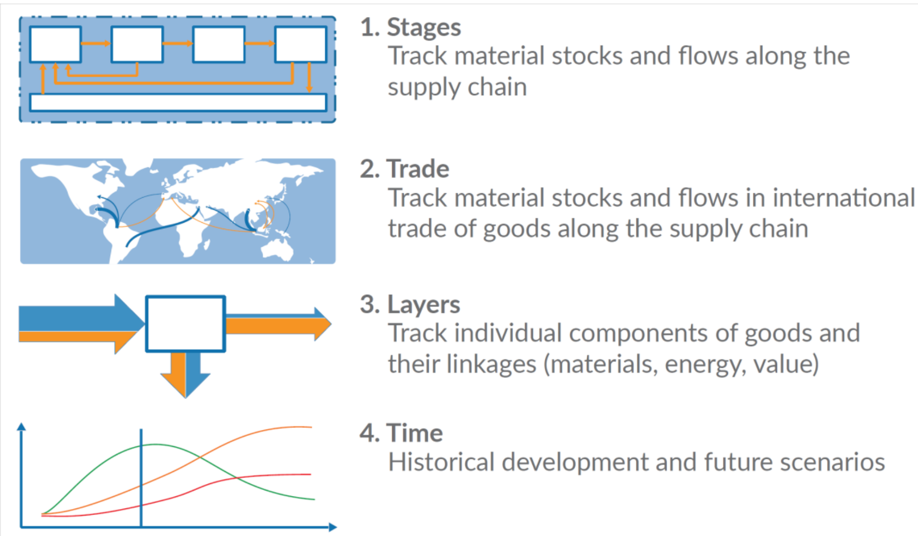

Figure 3: The 4 dimensions of MFA according to Müller et. al. (paper 1)

In this thesis, the time dimension is particularly explored through advances in dynamic MFA methods, and by the explicit consideration of time-dependent inventories in the plant-level approach. The stages dimension is explored at different scales, from plant level to global level. Most papers used a multilayer approach, as shown in Figure 2. The trade dimension is not explicitly addressed in this thesis, even if some papers have a regional approach, and if paper 2 considers trade at a very local scale by tracking the exchanges of materials between the plant studied and the other plants and companies.

Paper 1 also introduces the seven conceptual components necessary to monitor the physical economy: systems, data, models & scenarios, uncertainty, visualisation, indicators, and strategy & decision support (Figure 4). These components form a hierarchy, figured by the pyramid, in the sense that the robustness of each component is limited by the robustness of the components underneath. A more thorough description of the MFA framework to monitor the physical economy is available in paper 1.

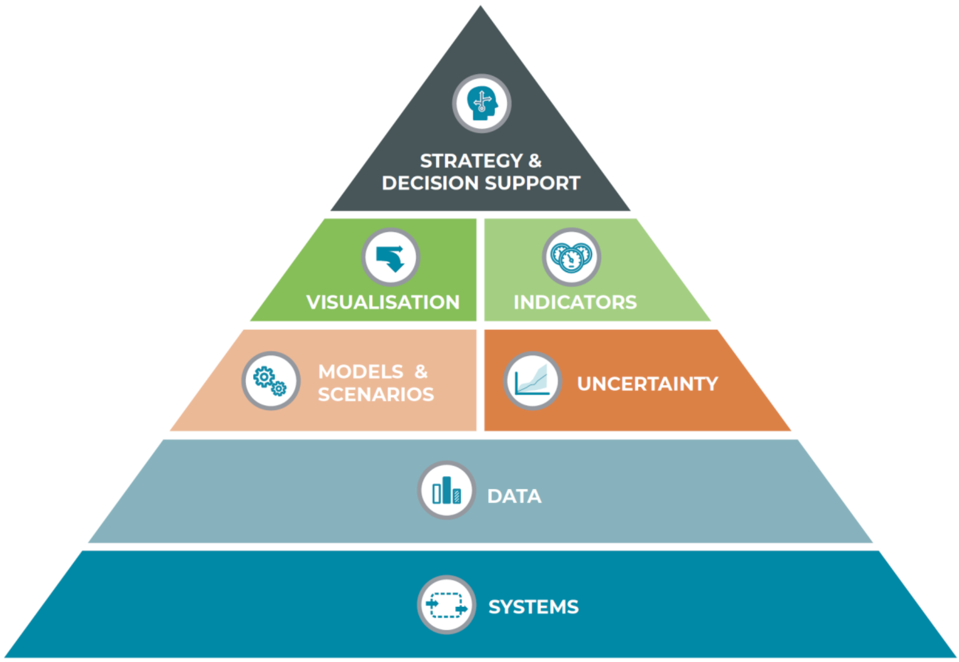

Figure 4: The 7 components for monitoring the physical economy according to Müller et. al. (paper 1)

2.2 Multilayer Plant-Level MFA and Physical Accounting

In the physical accounting framework based on plant-level MFA developed in paper 2, the concept of stages and layers (in this case, total mass, aluminium, and carbon) is applied to the scale of a single industrial plant (Figure 5). The approach is otherwise based on the 7 components for monitoring the physical economy. The metabolism of the plant was first described with a system definition, which was then updated after interviews with plant personnel. The system definition is also helpful in the data collection phase: each data point must be connected to an identified stock or flow in the system, enriching the metadata. Besides, data collection efforts are guided by the system definition: data gaps are made explicit, and the mass balance principle enables identifying and quantifying missing flows or changes in inventories. The system was quantified for one year (2019): changes in inventories are explicit and added to the system as stock changes, in opposition with approaches that only consider in- and outflows. A qualitative uncertainty was then assigned to the parameters and assumptions used to quantify the system, which enables to assess the parts of the system that are more likely to be affected by poor data quality or a lower degree of system understanding. A sensitivity analysis was also conducted for some important flows that used parameters with a high uncertainty. The data was then visualised with enriched Sankey diagrams, mapping the flows of the different layers throughout the system, and linking the GHG emissions to the corresponding processes and raw materials. In addition to internal key performance indicators (KPIs), additional indicators were developed to quantify the raw material efficiency of the plant and draw comparisons between the two smelting lines in use in the plant. The results of this physical accounting can then be used for strategy and decision support. In this example, this was made possible through the connection between internal corporate performance indicators, carbon reporting, raw material use, and waste generation. It also enabled to quantify the mitigation potential of different systemic measures, which can be further used to design a strategy to reduce GHG emissions and improve the efficiency of the plant.

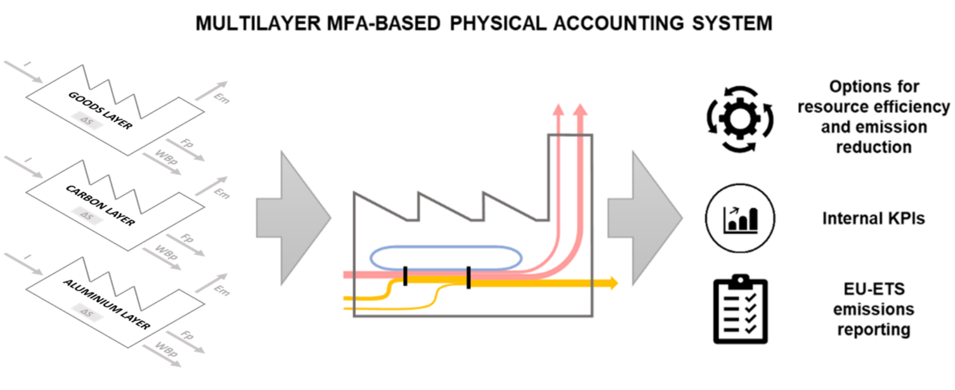

Figure 5: Example for the concept of a physical accounting system based on multilayer plant-level MFA (adapted from paper 2).

2.3 MFA AND STOCK DYNAMICS

2.3.1 Definitions: Towards a Common Language for Stock Dynamics

In order to increase the capacities of MFA models in the time dimension, dynamic models that consider the evolution of stocks and flows over time are needed. Paper 3 provides a conceptual framework for stock dynamics that can be applied to dynamic MFA and other disciplines, such as demography, systems dynamics, and population ecology. Figure 6 is a visual representation of the main elements of this framework. System variables (Stock (S), Inflows (I), and Outflows (O)) are linked together through the stock change via the intrinsic and balance equations. Other types of parameters can be used to link the different variables together: birth rates (b), death rates (d), growth rates (g) and lifetimes (L).

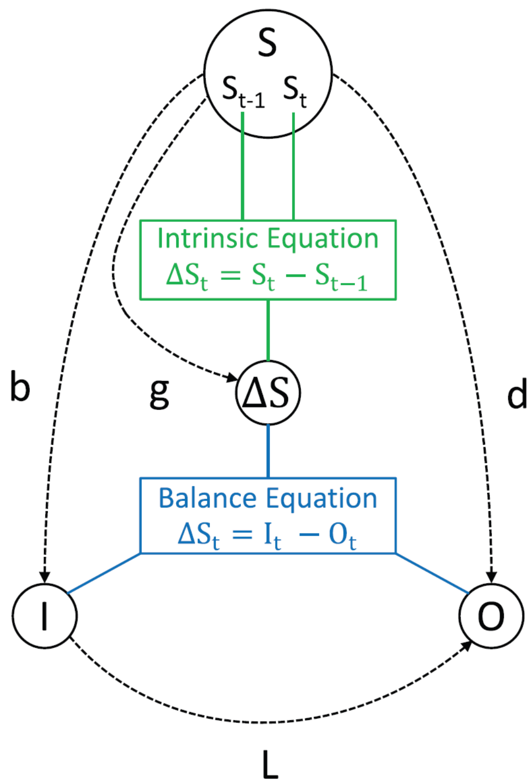

Figure 6: Basic relationships between system variables in stock dynamic systems (from paper 3)

2.3.2 Classification of Stock Dynamics Models

This framework can be used to classify the different models, depending on the system variables and parameters used to quantify it. An example of such classification is shown in Table 1. This allows us to visualise the classic dynamic MFA distinction between inflow-lifetime-driven (case 7) and stock-lifetime-driven models (Müller, Bader, and Baccini 2004) (case 15), but also other types of models that are mostly used in other fields of research. With this table based on an explicit mathematical framework, we can also visualize the data requirements of the different model classes, and potential limitations concerning the properties of system variables and parameters.

Paper 3 also introduces a new matrix-based formalism for stock-lifetime-driven dynamic models. The lifetime can be defined as a matrix L, so that outflows are derived from the inflows with the relation:

$$O = IL$$

Using the balance equation, we can express the stock change as a function of Inflows and Lifetime (with $\mathbb{I}$ the identity matrix):

$$\Delta S = I - OL = I - IL = I(\mathbb{I} - L)$$

Under the condition that $(\mathbb{I} - L)$ has full rank (all its diagonal elements are greater than zero, which should be verified in practice if the time step of the model is correctly defined), this can be written:

$$I = \Delta S(\mathbb{I} - L)^{-1}$$

Since the stock is directly linked to the stock change through the intrinsic equation, this equation can be used to solve stock-lifetime-driven models directly from the evolution of the stock and the lifetime. Since the $\mathbb{I} - L$ matrix is by construction upper-triangular, it can be inverted efficiently. Solving a stock-lifetime-driven model then theoretically only takes N (the number of periods in the model) extra arithmetical operations than solving the corresponding inflow-lifetime-driven model.

Table 1 – Classification of Stock Dynamics Models (Paper 3).
The system variables can be determined by combining flow and stock measurements with no model-approach equation (green), one model-approach equation (blue), or two model-approach equations (orange).

Case	Variables & Initial Stock				Parameters				Remarks
	$\boldsymbol{I}$	$\boldsymbol{O}$	$\boldsymbol{S}$	S_0	b	d	g	L	
Parameter-free Models									
1	■	■		■					For (1), it suffices to know the stock at some point in time t, which
2	■		■						
3		■	■						
1-Parameter Models									
4	■				/ ■				does not calculate O_T and
5	■			■		■			
6	■			■			■		
7	■			* ■				■	
8		■				/ ■			does not calculate I_T and
9		■		■	■				
10		■		■			■		
11		■		* ■				/ ■	only works if L is
12		* ■						/ ■	only works if a fraction of
13			■		■				
14			■			■			
15			* ■					// ■	cohort composition of S_0
Initial-stock-driven Models									
16				■	■	■			
17				■	■		■		
18				* ■	■			■	
19				■		■	■		
20				* ■		/ ■		■	
21				* ■			■	// ■	

* Cohort information required
/ Inverse relation must exist
// Inverse of $\mathbb{I} - L$ must exist

2.4 New Dynamic MFA Approaches

As carbon emissions keep increasing, future scenarios to remain below limited levels of global warming rely more on more on drastic measures. There is a need to adapt the dynamic MFA methodology to be able to model those and enrich the portfolio of interventions considered. For instance, a combined lifetime-leaching approach enables the modelling of the potential early replacement of the least efficient archetypes of the built environment. Product-component models allow us to detect potential cases of planned obsolescence. Conversely, they also enable to better investigate new strategies for lifetime extension, including component reuse or replacement. Finally, multilayer models with high sector-specific resolution in scenario parameters enable to better analyse the effects on material demand and associated emissions of the sustainable transitions in different sectors of the physical economy.

2.4.1 Use of hazard functions in dynamic MFA models

The definition of lifetime functions and distributions is an important part of dynamic MFA modelling. After choosing a lifetime distribution, the modeler needs to choose a lifetime distribution function to implement it in the model. Commonly used lifetime distribution functions in dynamic MFA are the probability density function (pdf), its integral the cumulative density function (cdf), and the survival function (sf), defined as $1 - sf$ (see Figure 7). Especially convenient is the sf, which directly links the inflows to the stock by cohort following equation (i), which simplifies calculations for both stock- and inflow-driven models. This, combined with the existence of ready-to-use open-source scientific packages (such as the scipy library in python) that ensure a convenient and fast computation, has led to the choice of using the sf in the ODYM software (Pauliuk and Heeren 2020).

However, in this thesis, a discrete hazard function is defined to facilitate the implementation of complex dynamic MFA models. This function is adapted from the continuous hazard function (or failure rate) commonly used in reliability engineering and survival analysis (Finkelstein 2008). In this example, $S(t, c)$ is defined as the remaining stock of a cohort c **at the end** of year t (or at the beginning of t-1). It can be calculated from inflows of cohort c $I(c)$ using the survival function of the chosen lifetime distribution, $sf(t,c)$:

$$S(t,c) = I(c) * sf(t,c) \qquad (i)$$

$$S(t-1,c) = I(c) * sf(t-1,c)$$

So, if $sf(t,c) \neq 0$ (which should be verified in practice, otherwise the stock-driven model cannot be solved) , $\forall\, t > 0$:

$$I(c) = \frac{S(t-1,c)}{sf(t-1,c)} \qquad (ii)$$

and $O(t,c) = S(t,c) - S(t-1,c)$

So:

$$O(t,c) = I(c) * \left(sf(t,c) - sf(t-1,c)\right) \qquad (iii)$$

By combining equations (ii) and (iii):

$$O(t,c) = S(t-1,c) * \frac{sf(t-1,c) - sf(t,c)}{sf(t-1,c)}$$

We define the hazard function $hz(t,c)$ as:

$$hz(t,c) = \frac{sf(t-1,c) - sf(t,c)}{sf(t-1,c)}$$

This hazard function can be used to calculate the outflows of a cohort during a given year from the remaining stock of this cohort at the beginning of the year:

$$O(t,c) = S(t-1,c) * hz(t,c)$$

The relationship between the probability density function of the lifetime distribution, $pdf(t,c)$, and the survival function, is given by:

$$sf(t,c) = 1 - \int_{-\infty}^{t} pdf(u,c)\ du = \int_{t}^{\infty} pdf(u,c)\ du$$

Therefore,

$$sf(t-1,c) - sf(t,c) = \int_{t-1}^{\infty} pdf(u,c)\ du - \int_{t}^{\infty} pdf(u,c)\ du$$

$$sf(t-1,c) - sf(t,c) = \int_{t-1}^{t} pdf(u,c)\ du + \int_{t}^{\infty} pdf(u,c)\ du - \int_{t}^{\infty} pdf(u,c)\ du$$

$$= \int_{t-1}^{t} pdf(u,c)\ du$$

Thus, the hazard function could be rewritten:

$$hf(t,c) = \frac{\int_{t-1}^{t} pdf(u,c)\ du}{sf(t-1,c)}$$

This is a discretization of the more commonly used definition of the hazard function:

$$h(t) = \frac{pdf(t)}{sf(t)}$$

This hazard function h defines the instantaneous force of mortality at time t. Since in dynamic MFA, time is usually discretised, and stock is only measured at given time intervals (e.g., every year), the discretized hazard function hf is more convenient to use.

There are some advantages of using the hazard function instead of the usual survival function in MFA, especially in cases:

- When only the initial stock and its cohort composition is known, but nothing else about the past. This is the case for example when the data used in the model comes from an extensive survey of the population, building stock, vehicle fleet, etc. The modeler has then a good understanding of the stock composition at a given point in time, but not of the historic inflows.
- When the size of the stock at time t might have been modified in the past by an external factor not captured by the lifetime distribution of the model (combined leaching-lifetime approach, component failure, reuse, accidents, import/export or immigration/emigration). In these cases, the initial cohort size is no longer representative of the remaining value of the stock, so the formula $S(t,c) = I(c) * sf(t,c)$ can no longer be used.

The hazard function might also facilitate the interpretation of the results in some cases. For instance, for a normal distribution, the hazard function is increasing exponentially indefinitely (Figure 7), which gives a better representation of the actual probability of reaching end-of-life for aged products or individuals. It also allows for a "purer" modelling of stock-driven models, where only the stock is used in the calculations, never involving the initial inflow. However, in simple cases, it remains easier to use the survival function, or the previously defined matrix relationship $O = IL \Leftrightarrow I = \Delta S\,(\mathbb{I} - L) - 1$

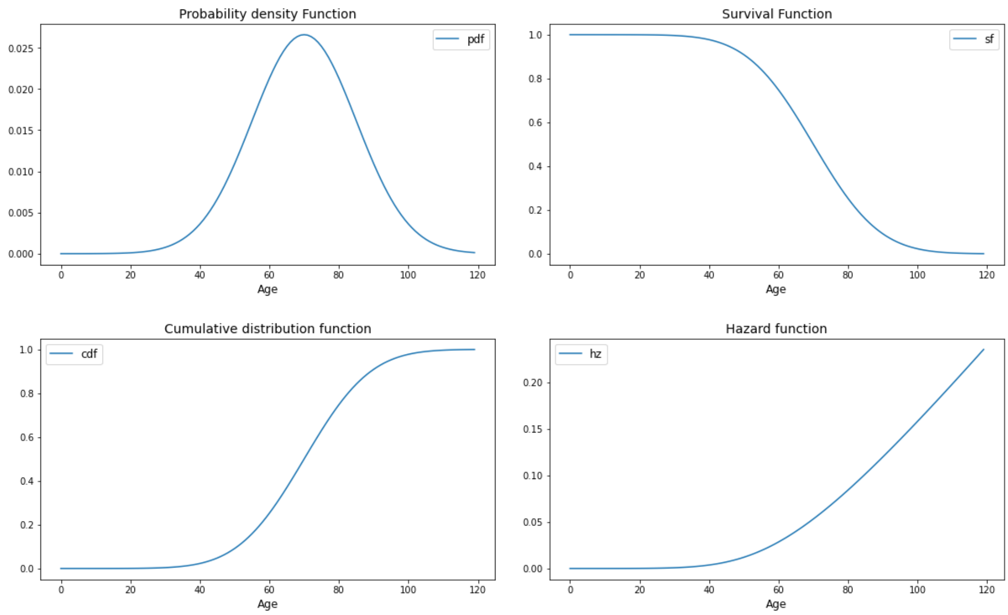

Figure 7: Example of several lifetime distribution functions for a normal distribution with a mean of 70 years and a standard deviation of 15 years

2.4.2 Dynamics of Product-Component Systems

Hazard functions are particularly useful in the case of product-component models. This class of models aim at describing the dynamics of systems composed of a main product and one or several components. Figure 8 shows a generic system definition in the case of a simple system composed of one product and one component.

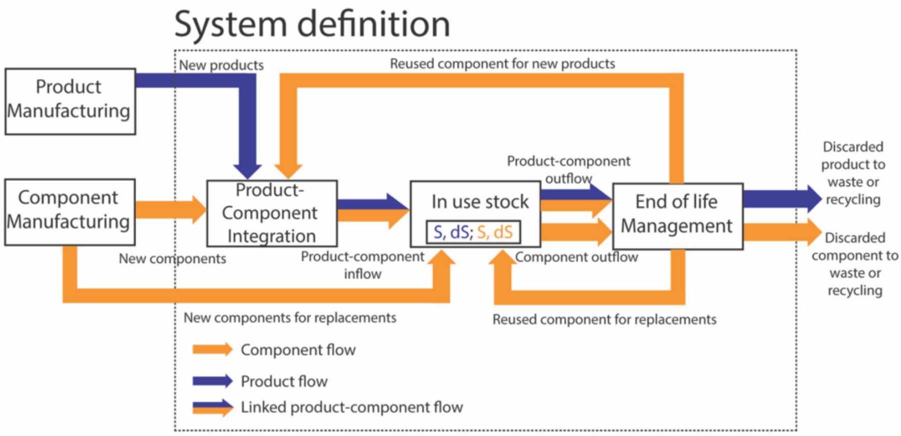

Figure 8: General system definition for a generic product-component system (from paper 4).

Figure 9 shows the classification of 12 elementary cases for product-component models. They differ depending on the existence of a lifetime for the product and the component, and on assumptions made about the potential replacement of defect components, or the reuse of functional components from failed products to replace failed components in other products. The description of each case and examples for applications are detailed in paper 4. An application of this framework is also found in paper 5, where a different lifetime is used for electric vehicles and their batteries and different battery replacement scenarios are considered.

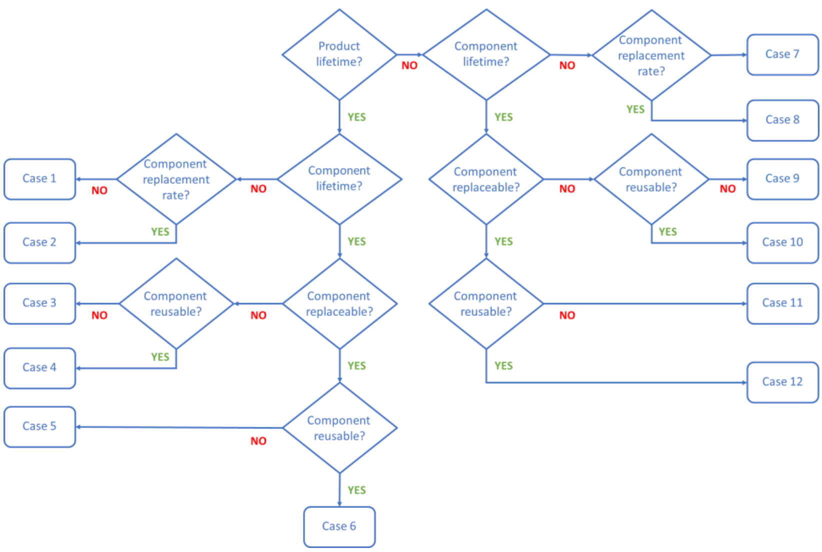

Figure 9: General classification of product-component models in 12 elementary cases (from paper 4).

2.4.3 Combined Lifetime-Leaching Models

In the previously described frameworks, death rate or leaching (case 14 in Table 1, case 7 in Figure 9: General classification of product-component models in 12 elementary cases (from paper 4).) and lifetime (cases 7, 11, 12, 18, 20, 21 in Table 1, cases 1-6 and 9-12 in Figure 9) models are presented as fundamentally different elementary cases. Leaching models are usually used for the sake of simplicity under certain conditions (Van der Voet et al. 2002), or when the phenomenon leading to outflows is mostly age-independent (such as leaching, hence the name, or accidents). In other cases where that the time span between inflows and outflows follows a robust statistical pattern, lifetime models are usually preferred (Melo 1999; Lauinger et al. 2021). However, it might be interesting to combined lifetime and leaching models in certain cases. This is for example the case for the bi-component Gompertz-Makeham law of mortality used in demography (Makeham 1860; Missov and Lenart 2013), which contains an age-dependent component (representing the increasing mortality due to ageing with an exponential function, similar to a lifetime model) and a constant component (representing accidents and causes of mortality not related to ageing, similar to a leaching model). In the study of the built environment, such an approach is useful to model transitions of the SEM, where products are retired before reaching their normal end-of-life in order to replace them with more sustainable alternatives. It can be used to model e.g., a ban of fossil fuel vehicles to accelerate the electrification of the transport sector, or a selective demolition of the least energy-efficient archetypes in the building stock to accelerate the effects of renovation and stricter construction codes, as was done in paper 7. A more detailed algorithm for the implementation of a lifetime-leaching approach is described in the supplementary information of paper 7, where the model was also refined to only affect specific cohorts of the building stock and consider the effects of renovations.

2.4.4 Scenario analysis based on the development of new products and technologies

The use of aluminium and other metals in products depend on their characteristics, which are changing over time. To better understand the material requirements of the transitions towards a sustainable SEM, it is necessary to develop dynamic MFA models with a high resolution on the characteristics of products in the in-use stock, using different archetypes and parameters to capture the changes in material composition, energy efficiency and carbon footprint. Papers 5, 6 (passenger cars), and 7 (buildings) all use a multilayer lifetime-stock-driven approach with a high resolution on in-use stock characteristics. Figure 10 shows an example of such a system definition, illustrating the different layers, dimensions for characteristics of the stock and corresponding archetypes.

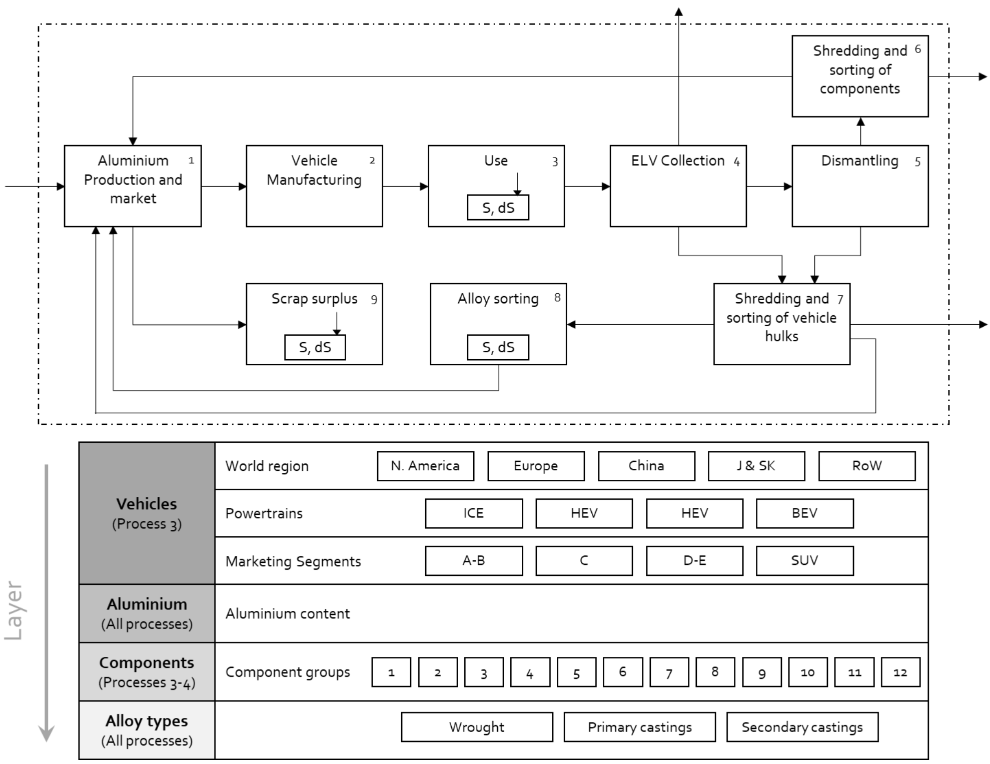

Figure 10: Example of a multilayer dynamic MFA system definition for aluminium use passenger cars, with high resolution to describe the different archetypes in the in-use stock (from paper 6)

Simulating the changes in the detailed composition of stock in the future is a data-intensive task that relies on many assumptions and scenarios. Fortunately, the recent development of open source dynamic MFA software, such as the ODYM framework (Pauliuk and Heeren 2020), facilitates the computation of a large number of scenarios across several system dimensions. Scenarios can be developed based on different future projections for the evolution of some key parameters in the system. For instance, in paper 6, all the combinations of 3 to 4 projections each for 8 parameters generate a total of 8 748 scenarios. Such a quantitative approach allows to test the effects of more parameter changes on the overall system and explores a wider solution space for future scenarios than a more classical one-factor-at-a-time (OFAT) approach. While not being a formal uncertainty or sensitivity analysis *per se*, this approach enables to design more robust future scenarios that consider a wider range of possibilities and therefore to better understand the impact of changes in parameters. Figure 11 is an example of results that can be generated with this method. Figure 11 a) shows all model runs for all of the 8 748 scenarios for aluminium demand, using transparency. Figure 11 b) shows the corresponding statistical distribution for three chosen years, which enables the visualisation of the median scenario and the likely range of the future demand.

New visualisations can also be created: for instance, for papers 5 and 6, interactive Sankey diagrams that allow the user to visualise the evolution of the cycle over time and for the different scenario parameters have been developed (the code for these applications is available in the supplementary information for these papers). According to the pyramid structure of the components of MFA (Figure 4), these interactive visualisations can serve as a bridge between the model results and decision makers and foster the use of MFA as a tool for strategy and decision support.

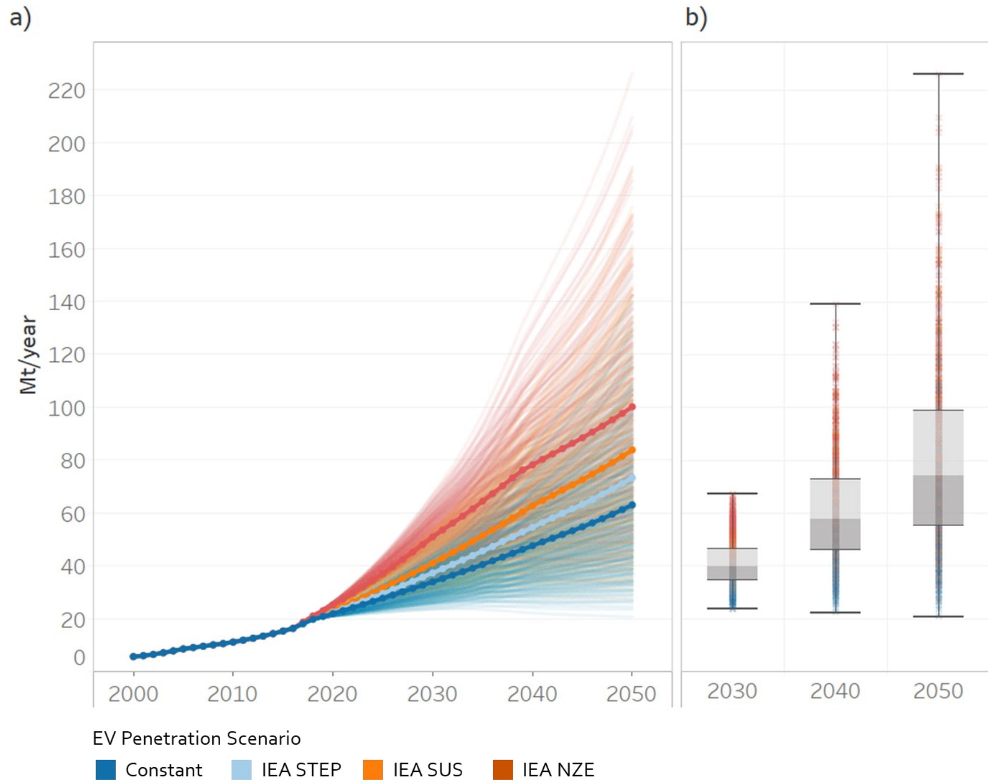

Figure 11: Future scenarios for aluminium demand in passenger cars (from paper 6)

3 Main findings and reflexions on the research questions

3.1 Question 1: How can metal cycles and their emissions be monitored more effectively based on mass and energy conservation principles?

In paper 2, we showed that different methods for reporting and monitoring emissions of metal cycles correspond to different aims. If the current carbon accounting and reporting schemes such as the EU ETS enable a relatively simple and fast way to quantify emissions of industrial plants, they suffer from structural weaknesses that do not make them a suitable strategy and decision support tool. They also result in a fragmented understanding of the production sites, making them unsuitable for comparisons and systemic optimisation. Physical accounting based on plant-level MFA has the potential to reconcile internal performance indicators with mandatory climate reporting. Furthermore, the generated insights can be used to improve the data quality (by use of the mass balance principle) and the relevance of simulation models, and to align climate policies for industrial sites with future projections for metal cycles and associated emissions. This physical accounting framework based on a robust system definition can serve as the foundation for a comprehensive monitoring system for the physical economy.

The generalisation of such physical accounting systems can be seen as expensive but can instead result in cost-savings: current carbon accounting practices are already expensive and do not result in meaningful indicators that can be used by plant managers to monitor the overall performance of the plants, which requires to maintain separate reporting systems in parallel. Besides, if in this thesis, we mostly focused on the use of this framework for monitoring emissions, further applications exist. For instance, the systematic multilayer cartography of waste flows (Figure 6 in paper 2) can help generating value from waste by identifying and quantifying valuable waste fractions that could be valorised better with some operational changes.

This approach can also be extended further by the use of industrial control data to quantify the system (Gonzalez Hernandez et al. 2018). The use of a highly granular system definition can help providing the metadata needed to correctly position data from automatic sensors, while data reconciliation algorithms could help compute and resolve material and energy balances of processes and plants in close to real time, helping with performance monitoring and management of raw materials, energy, and waste. With the development of digital twins for factories, advanced monitoring systems could then be coupled to simulation tools which will allow plant managers to quickly react to changing conditions, such as a change in raw materials composition.

As traceability becomes an increasingly important issue for metals, robust monitoring systems can also play a role in increasing the transparency of the operations of industrial plants and in identifying products that follow certain specifications with regards to carbon emissions, working conditions, local environmental impacts or human rights. For aluminium, the recent efforts towards a decommodification of the industry, with initiatives such as the Aluminium Stewardship Initiative or the push of certain companies to promote different product qualities (e.g., with lower carbon footprint or higher recycled content), could benefit from a more transparent and systematic approach to monitor the environmental performance of industrial plants.

3.2 Question 2: How can we facilitate the evaluation of transition strategies for metal cycles using refined simulation models?

This thesis has its main focus on scenario analysis based on dynamic MFA, which is a relatively new field. Dynamic stock models have been used far longer in other fields (e.g., demography, ecology, forestry…), sometimes for centuries. With the framework developed in paper 3, we aimed to define a common language and mathematical formalism for models studying the dynamics of stocks within systems, in order to strengthen connections between these different fields and foster multidisciplinary learning. We developed a classification that helps modellers to better understand similarities and differences between different elementary model classes for stock dynamics.

This classification also made it easier to identify new needs. For instance, stock-driven MFA models that use a lifetime to compute outflows usually do not distinguish between the different causes for a product to reach end-of-life. They also tend to consider a product as a single entity, while in reality it is often made of a large number of different components. For instance, a car is composed of many different parts that may fail and be replaced during its lifetime, but also lead to its scrappage if a repair is no longer viable compared to the resulting economic value of the car. The framework we presented in paper 4 is a first step towards better representing interactions between products and their component in simulation models. It allows the modeler to use a different lifetime for the product and a component, as well as different assumptions concerning replacement and reuse which facilitated the evaluation of circular economy strategies. We presented as an example the case of EVs and their batteries, but this approach could be used in many other applications, for example to improve the modelling of building renovations.

This framework is however very simplified and considers only one component. Future applications should aim at generalising this approach to systems that contain several components. In this case as well, a multidisciplinary approach is likely to yield results, as such models have already been developed and used in the field of reliability analysis. This approach is particularly promising for dynamic models of new products and technologies, whose lifetime would have to be estimated in collaboration with the engineers that design them.

The combined lifetime-leaching approach developed in paper 7 allows us to model the effect of a broader set of interventions to accelerate the transition to a more sustainable SEM. By targeting and replacing the least performant archetypes of a building stock, vehicle fleet, or other products, policies can accelerate the rate of change compared to a natural replacement rate. However, our first results suggest that the benefits of such a radical approach are limited, and that it should be restricted to extreme cases. In the case of the building stock, extensive renovation and adjustments in lifestyle make it possible to reach similar results, with a limited material demand compared to a scenario with increased demolition. In paper 7, the emissions of material extraction and production were not considered but are likely to reduce or even offset the benefits of the premature demolition. In this case, premature demolition was used as an extreme example of what is theoretically possible to achieve with a faster renewal of the stock, but further research using a combined lifetime-leaching approach should analyse simultaneously the energy and material demand.

Indeed, increasing public and political awareness of climate change issues might lead to the adoption of more radical policies to accelerate the transition to a sustainable SEM. However, the risk is that the transition itself will require considerable amounts of energy and raw materials, and challenge material cycles to the point of creating unacceptable environmental and social impacts. A lifetime-leaching approach enables a better modelling of the effect of such fast transition, by also illustrating the consequences on material and energy demand of retiring products and infrastructures before their design lifetime.

Stock-driven models have been successfully used in the last 20 years to build forecasts for material cycles. However, as shown in papers 5, 6, and 7, future scenarios are highly dependent on assumptions made on the characteristics of products in in-use stocks. These characteristics can change over time and across different product archetypes. It is therefore important to have a large enough data foundation to cover this complexity in enough detail and consider multiple scenarios for future evolution. For instance, in paper 6, the aluminium content in cars is changing depending on the archetype (EV vs. ICEV, small vs. bigger cars), but also over time to reflect the increasing use of aluminium for light weighting. This characteristic is fundamental in explaining the difference in results with other publications that only consider one or the other, and therefore tend to underestimate the cumulative effect on the total future demand for aluminium in cars.

The scenario-rich approach used in papers 5 and 6 makes use of new dynamic MFA software to compute a large number of parameter combinations to create future scenarios. This provides a better understanding of what a likely future might be by exploring a larger solution space. The influence of the different drivers on the system is also easier to quantify, especially since the effects of combined changes can be represented. However, this approach could be complemented by a more formal sensitivity and uncertainty analysis, even if this task is made harder by the constraints inherent to a dynamic model: the intrinsic relation that ensures the continuity of system variables over time further restricts the evolution of the different parameters, making traditional uncertainty analysis methods harder to apply, notwithstanding the difficulties related to computation time and the amount of data generated.

3.3 Question 3: How can we apply these monitoring and simulation tools to the aluminium cycle and its emissions?

3.3.1 Monitoring GHG emissions of the aluminium cycle

The application of the physical accounting framework developed in paper 2 to an aluminium smelter delivered promising results. Mapping the flows of total mass, aluminium, and carbon within the plant enabled the quantification of GHG emissions and the identification of the responsible source streams and processes. Compared to classical carbon reporting approaches, this higher granularity in the monitoring allows plant managers to better understand the determinants of the emissions of the plant and therefore identify the most effective reduction measures. The methodology is also more transparent and enables easier comparisons between different plants: a typical example for aluminium smelters is that some plants do not have on-site anode baking facilities, making their direct GHG emissions lower for a similar quantity of aluminium produced. Our approach would allow corporate and government decision makers to use the provided system definition to make comparisons on similar premises. A generalisation of this framework would also greatly improve the statistics on the overall GHG emissions of the aluminium cycle. With an explicit system definition, it would be easier to connect the different scales to build a bottom-up monitoring system of the global aluminium cycle and its GHG emissions.

3.3.2 Consequences of increasing demand for aluminium in transport applications

The results of papers 5 and 6 clearly show that the demand for aluminium in transport applications will significantly increase in the coming decades, driven by the use in batteries and their casings, and increasing light-weighing in other car components. Demand for aluminium in cars is likely to increase by a factor 3 to 5 between 2020 and 2050. The demand for other battery materials, such as lithium, cobalt, nickel, and manganese, will also increase in large enough proportions to deeply reshape their respective global cycles. The scope of these studies was limited to passenger cars, but similar trends can be expected for trucks, busses, and other means of transport, increasing further the total demand.

This work highlights the need for comprehensive policies for a sustainable use of materials in transport applications. Most current policies are focusing on improving fuel efficiency and reducing emissions of GHGs and pollutants in the use phase. As the electrification of the transport sector increases, it becomes more and more necessary to focus on monitoring and reducing the impact of the material production and manufacturing phases. In paper 6, we showed that many policies aiming at reducing the use-phase emissions of cars or accelerating the penetration of electric vehicles (EVs) or plug-in hybrid electric vehicles (PHEVs) lead to an increase in the material footprint of the cars. Recent initiatives such as the European Battery Directive (Halleux 2022) aim at limiting the material footprint of batteries, but this proves challenging for aluminium for several reasons: (i) these policies tend to focus more on other battery-specific materials, such as nickel, cobalt, lithium, or manganese; (ii) aluminium is used both in the batteries and in other car components: they are usually covered in separate directives, making it hard to design comprehensive policies targeting reduction of the total carbon footprint of aluminium; (iii) carbon footprint is a limited metric that allocates emissions to materials and products but does not assess the performance of the overall system; (iv) aluminium is produced and used globally in a wide range of products, which increases the risks of carbon leakage and burden shifting to other sectors, making it challenging to design robust and effective calculation methodologies and policy targets.

Indeed, other sectors that were not considered in this thesis are also likely to experience an increase in aluminium demand in the near future. For instance, the use of aluminium for electronics and cables is expected to increase as a substitute to copper. The transition of the energy sector towards more renewable might generate a considerable demand for aluminium in photovoltaics panels (Lennon et al. 2022). Packaging applications are also increasing rapidly, and the building sector is expected to keep representing a large share of the aluminium demand. Models investigating the totality of the end-use sectors would enable a better quantification of the total aluminium demand and are needed to understand the exchanges of scraps between different sectors. However, sufficient single sectors resolution is needed to correctly understand the drivers of future aluminium in specific applications. Failing to do so will lead to high uncertainties and is likely to result in an underestimation of the aluminium demand. For instance, studies with a larger scope, e.g., from (Liu, Bangs, and Müller 2013) or Pedneault et al. (2021), tend to omit fundamental transformations of the passenger car sector, which results in lower estimates for future aluminium demand than what was simulated in paper 6. This illustrates the potential for modular modelling frameworks that aggregate information about material cycles at different scales, so that smaller scales models can inform simulations with a larger scope.

3.3.3 Options for reducing GHG emissions from aluminium production

3.3.3.1 Potential for Increasing secondary production

Increasing the share of secondary production is one of the most effective measures to reduce GHG emissions of the aluminium production sector. However, the future share of secondary production in the total demand is inherently limited by the stock dynamics of the aluminium cycle. The demand for aluminium has been increasing faster than for any other major metal in the last 25 years (Rasul and Hertwich 2022). This trend is continuing, and all categories of aluminium final products are expected to experience a fast increase in demand in the coming years. This situation, combined with the fact that some major applications of aluminium (such as buildings and vehicles) have a comparatively long lifetime, means that the delay between inflows and outflows will limit the contribution of recycling as long as the demand keeps growing.

Besides, as shown in paper 6, recycling all the available scrap will be a challenge in the future. The demand for wrought alloys is growing, while the electrification of the transport sector leads to a lower demand for secondary castings. The high concentration of alloying impurities and alloying elements in secondary castings implies that remelting secondary castings or mixed-alloys scrap will require too much dilution with primary aluminium to reach the desired composition for wrought alloys, leading to a risk for a scrap surplus which would limit the climate mitigation potential through recycling (Modaresi, Løvik, and Müller 2014). Paper 6 demonstrated that the size of the future scrap surplus is primarily driven by the electrification of the vehicle fleet and can reach levels as high as 20-60 Mt/yr in 2050 in the fastest electrification scenarios.

This analysis only considers the scrap use in the passenger car sector. This could mean that it neglects the potential for using more secondary castings in other sector, but since the automotive sector is currently acting as a sink for the scrap from other sectors (Modaresi and Müller 2012), this assumption actually leads to an underestimation of the scrap surplus issue. The fact that closed-loop recycling of pre-consumer scrap was assumed to be unproblematic also contributes to make the results a conservative estimate for the scale of future scrap surplus. However, the inclusion of other sectors would help reducing uncertainties surrounding this problem. New applications from post-consumer scrap might be found in other sectors, especially since a future scrap surplus is likely to lead to a greater differential between the price of old scrap and primary aluminium.

This price differential is the main argument to consider a fast penetration of alloy-sorting technologies (which are not used at industrial scale for post-consumer-scrap today) and/or an increased dismantling of aluminium parts before shredding. Paper 6 has shown that this could greatly alleviate the effects of the switch from castings to wrought alloys: the demand for secondary castings will remain high enough in the future to absorb the generated scrap, assuming perfect alloy-to alloy recycling. However, the economics of a generalisation of these technologies at a larger scale remain unknown, and a comprehensive redesign of the aluminium recycling system will require a greater collaboration between actors operating at different stages of the value chain. For instance, car manufacturers and original equipment manufacturers (OEM) could improve their designs to facilitate dismantling and reduce the number of alloys used. A tighter connection between manufacturers, recyclers and scrap dealers is also needed to ensure that scrap fractions of suitable qualities to make new products are kept separated to avoid cascading.

In paper 6, we demonstrated that increasing the average lifetime of cars will also help to delay and reduce the size of the scrap surplus. EVs might indeed end up with a lower lifetime than internal combustion engine vehicles (ICEVs) because they are relatively simpler, with fewer moving parts and mechanical constraints. This could mean that the technical lifetime of EVs should in theory be longer than for ICEVs, if not limited by the lifetime of their batteries. However, car lifetimes are in general difficult to estimate, as trade of second-use vehicles between countries is not well monitored: a car apparently leaving the in-use stock of a given country could still be in use somewhere else. For EVs, this problem is made worse by the fact that there is not enough historic data available to assess the practical lifetime of this new technology, especially concerning the real lifetimes of batteries, which are likely to increase with the larger capacities and new battery technologies. Paper 4 uses a component-model framework to investigate how different assumptions concerning car and battery lifetimes and options for replacement and reuse influence the demand for new products. Circular economy strategies that foster the replacement and reuse of batteries have the potential to increase the average vehicle lifetime, under the assumption that the health status of used cars and batteries (and hence the remaining potential lifetime) can be correctly assessed. Nevertheless, legal and practical challenges related to the reuse of batteries are currently limiting the implementation of these strategies. Furthermore, policies to accelerate the electrification of the fleet tend to make new EVs cheaper, reducing the incentives to repair and reuse older cars and batteries.

Finally, research is still conducted to develop new technologies to upcycle automotive scrap. The potential of solid-state electrolysis to obtain high purity aluminium from post-consumer scrap has been demonstrated at lab scale (Lu et al. 2022) and industry claims that a larger scale implementation is possible in the short term (Alcoa 2021). However, the real energy consumption of this process is difficult to assess. First estimates are in the range of 50% of the energy requirements of primary production (Lu et al. 2022), which is still about 10 times the energy needed for classical remelting. In the absence of new breakthroughs, dismantling and sorting should therefore remain the preferred options, at least in the short-term.

3.3.3.2 Potential for reducing emissions of primary production

Recycling alone will not be enough to mitigate the future GHG emissions from the aluminium sector: as significant volumes of primary production will be needed in the foreseeable future, mitigation efforts should also focus in reducing the impact of the primary route, especially in the smelting process.

The results from the plant-level study of a smelter in paper 2 show some potential for reducing direct GHG emissions. Improving the efficiency of the alumina reduction reaction and limiting air burn were shown to have a theoretical emission reduction potential of 7.1 % and 5.5 %, respectively. Changing the energy carrier from liquid natural gas to hydrogen in heating processes for anode baking and casting could also reduce the direct emissions by 4.2%, but this is not considering indirect emissions related to the production of hydrogen. Other measures such as reducing further the anode effect also had a small reduction potential. However, the industrial feasibility of these measures was not investigated, and the real potential is likely to be much smaller: marginal gains are getting harder to reach as the prebake-anode smelting technology is already mature and has benefited from decades of continuous improvement. Besides, the biggest contributor to direct GHG emissions from smelting is the oxidation of anodes during the electrolysis, which is part of the process and cannot be avoided with the current smelting technology.

A new smelting technology based on inert anodes could theoretically eliminate most direct emissions from the smelting process. Research on this topic has been going on for several decades, with mixed results, but recent developments tend to make a medium-term deployment of this technology plausible (He et al. 2021). Pilot plants are currently being developed (Svendsen 2022), but little is known on the practical results, especially concerning the capabilities of the anodes to remain completely inert. It is also expected that this technology would decrease the energy efficiency of the smelting process (Solheim 2018), meaning that its implementation would only make sense in plants that already have access to low carbon electricity sources. Besides, the extent to which it would be possible to retrofit inert anodes to existing pre-bake plants is crucial for the potential of this technology.

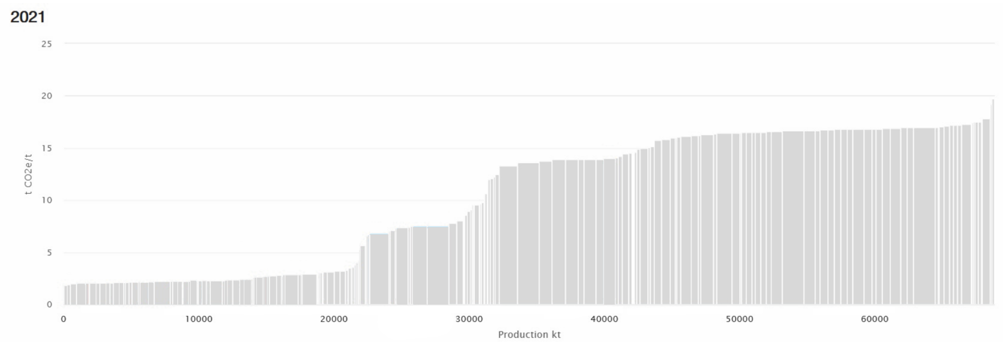

Figure 12: Production and emissions intensity for all 2021-operating aluminium smelters (Adapted from CRU 2022). *Each bar is representing a smelter. Emissions include scopes 1, 2, and parts of scope 3 (to account for smelters that do not have in-house anode production).*

Figure 12 shows the current distribution of the emission intensity of the global portfolio of aluminium smelters, showing large discrepancies between individual plants. These differences are caused mostly by the differences in electricity mix: lowest emitting smelters use hydroelectricity, while the most emission intensive ones use coal-based power. Electricity supply is indeed representing both the largest source of emissions and the largest potential to reduce the carbon footprint of the aluminium industry (Liu, Bangs, and Müller 2013; International Aluminium Institute 2021a). The differences in technology and age of the smelters are also playing a smaller role in these differences. Due to the long lifetime of industrial assets such as aluminium smelters (Figure 13), the penetration of inert anodes and the decarbonisation of electricity sources could be slowed down by the lock-in effect that the current stock of smelters represents.

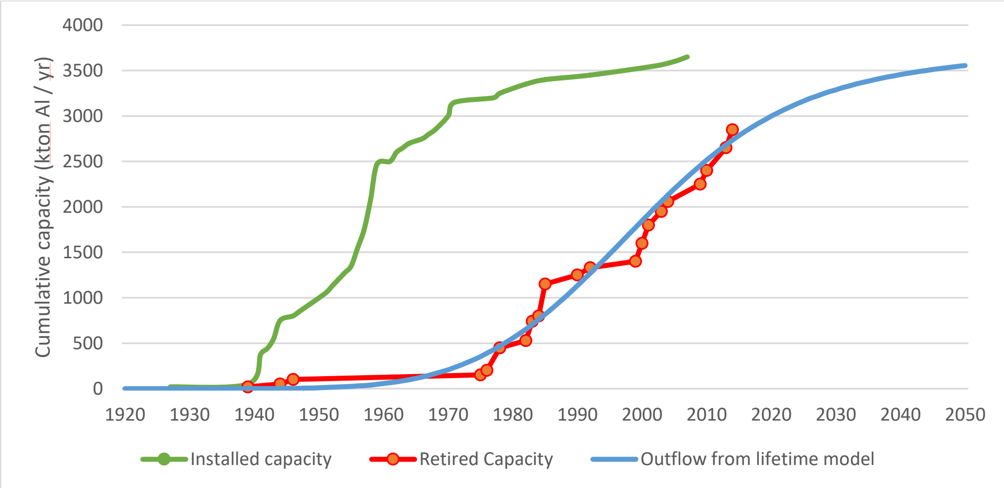

Figure 13: Penetration and retirement of the Søderberg smelting technology in North and South America. The blue curve is showing the outflows obtained from an inflow-lifetime-driven dynamic MFA model using a normally distributed lifetime with a mean of 42 year and a standard deviation of 15 years. Historic data from Barber and Tabereaux (2014).

Other parts of the aluminium value chain were not analysed in such level of detail in this thesis. Even if primary smelting is the single most important process for GHG emissions in the aluminium industry, there is also potential for improvements in other parts of the system that were not investigated. For instance, while the high aluminium ore grades make the emissions associated with bauxite mining almost negligible, alumina refining is responsible for 17-22 % of the overall carbon footprint of primary aluminium (International Aluminium Institute 2021b; Gautam, Pandey, and Agrawal 2017). Options for reducing this share exist, such as using electric or hydrogen boilers for steam generation, implementing mechanical vapour recompression, using fluidized bed calciners, or lowering the temperature of the digestion process. (Liu, Bangs, and Müller 2013; International Aluminium Institute 2021a; Mission Possible Partnership 2021; 2022). Secondary production only represents a fraction of the carbon footprint of primary production, and improvement potentials lie mostly on systemic measures to improve the overall use of scrap. However, direct emissions of secondary melting processes could also be reduced through the replacement of gas fired furnaces by electric or hydrogen powered furnaces.

4 Conclusions and Outlook

The focus of this thesis has been to design new tools to monitor and simulate metal cycles and their emissions with a higher granularity. With applications mainly focusing on different aspects of the aluminium cycle, we demonstrated some of the benefits that can be expected from a greater use of these tools. The policy and industry relevant insights that can be generated by these models can be a precious aid to design the metal cycles needed to build a more sustainable SEM. This last section is however focusing on three topics that were identified as important research areas to further improve our understanding and modelling of metal cycles in general and aluminium in particular.

4.1 Technology explicit models

Metal cycles are influenced not only by the current and future levels of in-use stocks in products, but also by the technological, financial, and human stocks within the metal industry. To better simulate future metal cycles, it is necessary to better account for their interactions with the rest of the SEM, such as investments, trade, needs for investments, technologies and infrastructure, land use, and jobs creation. Fixed capital stocks, lacking in traditional MFAs, could be included in dynamic models to account for how production systems evolve in relation to these assets, and to consider potential lock-in effects that could slow down the development of new technologies (Pauliuk, Wood, and Hertwich 2015). This would also facilitate the link with economic and larger scale models, while keeping the mass balance principle and higher degree of resolution that is lacking in most input-out and integrated assessment models.

For the aluminium cycle, an important question is how fast new technologies can be developed and replace old ones, especially in primary production. Indeed, new technologies tend to be implemented with a significant delay, since the replacement of old technologies is often not economic. Hypotheses on available technology and economical perspective allowed to estimate the potential for reduction in energy and emissions in primary aluminium production (Moya et al. 2015), while projections for future aluminium demand and associated impacts have been developed (Van der Voet et al. 2018). There are still large differences in energy efficiency among smelters (IEA

2009), so the replacement rate of old smelters will have an impact on the overall energy demand from aluminium production. Such numbers show an opportunity for decreasing the environmental impacts of the aluminium cycle through better technology (such as inert anodes), even if the extent of this improvement depends on how fast cleaner technology is implemented, depending on its availability and on investment choices. The industry expects a sharper increase of aluminium production in the two coming decades, with a CAGR in the range of 4%, which would require the construction of about 40-50 new smelters in addition to the replacement of old smelters (Nappi 2013). However, in the future, the need for new primary production capacity might be limited by the increasing amounts of scrap available, meaning that the penetration of new technologies will be greatly influenced by the growth pattern of in-use stocks. Besides, scenarios focusing on technologies improving energy efficiency should also consider the potential associated rebound effects (Sorrell 2009), which could be large in cases where power supply is the limiting factor of production.

These findings emphasize the need for a holistic dynamic and technology explicit model of the global aluminium cycle. Figure 14 is showing the example of a concept for such a technology-explicit model of the global aluminium cycle, which considers the stocks and lifetimes (according to Figure 13) of technological assets.

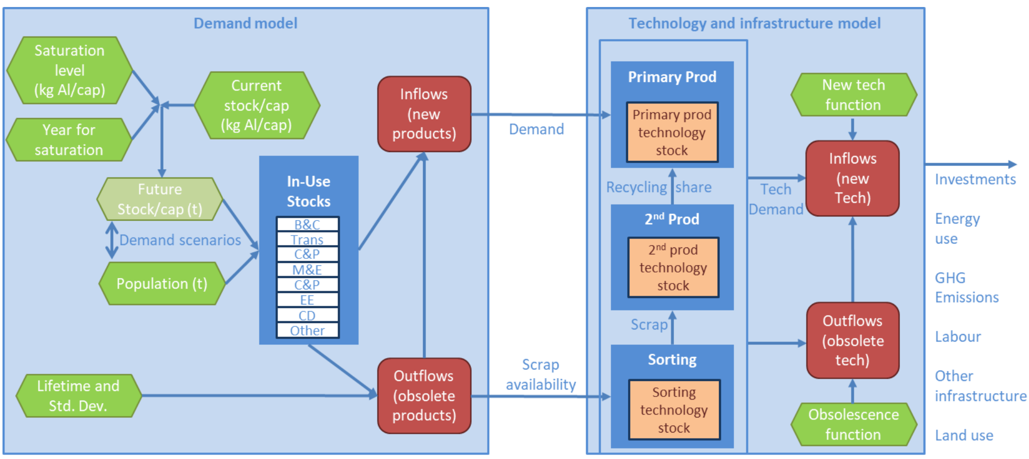

Figure 14: Concept for a technology-explicit model of the global aluminium cycle

4.2 COMBINING MATERIAL AND ENERGY EFFICIENCY

Furthermore, analysis of future scenarios using new technologies would benefit from an approach that considers simultaneously material and energy efficiency (Allwood et al. 2013). In this thesis, different papers have considered materials and emissions or energy and emissions, but not the three at once. This is an important limitation, as some reduction strategies might optimize one at the expense of the other: for instance, replacing old buildings by newer ones might be beneficial for the energy use of the building stock, but will require large quantities of materials. Conversely, increasing the yield of sorting and recycling processes over certain limits can lead to a higher material efficiency, but at the cost of a higher energy use. Global and country-level studies following this approach have already been conducted on the steel cycle, at the global (Milford et al. 2013; Gonzalez Hernandez, Paoli, and Cullen 2018), national (Allwood 2013) and plant level (Gonzalez Hernandez et al. 2018), showing the importance of introducing both energy and material efficiency measures to meet climate targets.

4.3 THE TRANSPORT – MATERIAL – ENERGY NEXUS

Material cycles are key elements to build a new sustainable SEM, and an important question is the quantities of materials (and corresponding energy and emissions) needed to realize the transition towards a more sustainable SEM. The scale of the transitions needed in the transport (Modaresi et al. 2014) and energy sectors in particular will require considerable amounts of aluminium and specialty metals to build the battery and renewable energy capacities needed in 1.5 degrees scenarios (Hertwich et al. 2015; Lennon et al. 2022). Mining and refining these materials will in turn increase the energy demand, which will have to be met with new renewable capacities, creating a feedback loop between material and energy demand. Figure 15 illustrates these feedback loops for aluminium. Future research on material and energy requirements of the decarbonisation of the transport and energy sectors should aim at better considering these effects. Studying the transport-material-energy nexus in a unified framework would allow modelers to quantify the additional amounts of materials and energy needed when considering feedback loops. Additionally, this could better illustrate the potential of demand-side or material efficiency mitigation strategies (such as reducing the size of cars or the demand for transport), which in addition to their benefits within the transport sector also yield energy and emission savings in the wider system.

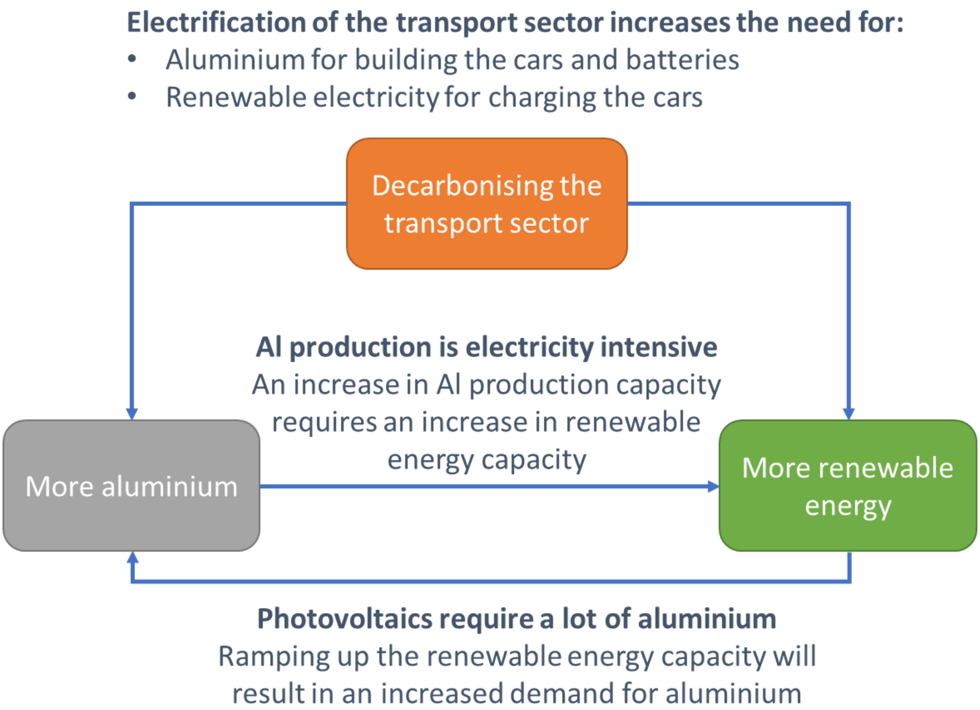

Figure 15: The transport-materials-energy nexus with the example of aluminium

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Paper 1

MAPS OF THE PHYSICAL ECONOMY TO INFORM SUSTAINABILITY STRATEGIES

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Paper 2

Systemic Approaches for Emission Reduction in Industrial Plants Based on Physical Accounting: Example for an Aluminum Smelter

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Article

Systemic Approaches for Emission Reduction in Industrial Plants Based on Physical Accounting: Example for an Aluminum Smelter

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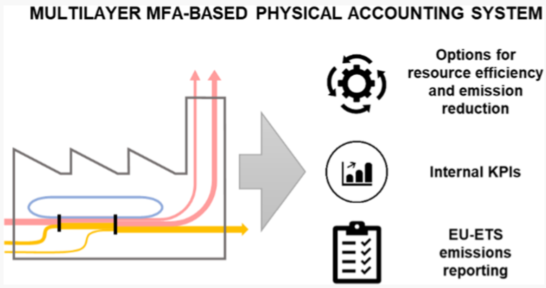

ABSTRACT: Greenhouse gas (GHG) accounting in industrial plants usually has multiple purposes, including mandatory reporting, shareholder and stakeholder communication, developing key performance indicators (KPIs), or informing cost-effective mitigation options. Current carbon accounting systems, such as the one required by the European Union Emission Trading Scheme (EU ETS), ignore the system context in which emissions occur. This hampers the identification and evaluation of comprehensive mitigation strategies considering linkages between materials, energy, and emissions. Here, we propose a carbon accounting method based on multilevel material flow analysis (MFA), which aims at addressing this gap. Using a Norwegian primary aluminum production plant as an example, we analyzed the material stocks and flows within this plant for total mass flows of goods as well as substances such as aluminum and carbon. The results show that the MFA-based accounting (i) is more robust than conventional tools due to mass balance consistency and higher granularity, (ii) allows monitoring the performance of the company and defines meaningful KPIs, (iii) can be used as a basis for the EU ETS reporting and linked to internal reporting, (iv) enables the identification and evaluation of systemic solutions and resource efficiency strategies for reducing emissions, and (v) has the potential to save costs.

KEYWORDS: *material flow analysis, carbon accounting, aluminum smelting, material accounting, material and energy efficiency, systems analysis*

■ INTRODUCTION

The industry sector contributed just over 30% of the global greenhouse gas (GHG) emissions in 2010,[1] and the aluminum value chain alone embodied in 2009 approximately 1.1% of the global GHG emissions, whereof 90% was associated with primary production,[2] which is expected to keep soaring for decades.[3] If global warming were to be stabilized at 2 °C above pre-industrial levels, the carbon intensity in the industrial sector would decrease by 60% in 2050 compared to 2010 levels.[4] Emission trading systems (ETS), such as the European Union ETS (EU ETS), are established to help fulfill this goal.[5] The EU ETS currently requires industrial installations from 28 sectors (including primary aluminum production) to account for their direct (scope 1) CO_2, N_2O, and perfluorinated compound (PFC) emissions, covering 45% of EU's total territorial carbon dioxide emissions.[6] A cap on these emissions was established at the EU level in 2013 (phase 3) and set to decrease by 1.74% each year and by 2.2% from 2021 onward (phase 4).[7]

Emission accounting is a prerequisite to any ETS to spot the biggest contributors, assign responsibility, and track performance evolution over time. Under the EU ETS, this is carried out following guidelines and methodologies issued by the EU,[8] which aim to standardize the accounting process but not to identify and evaluate emission reduction strategies. Industrial installations are only required to report their total direct GHG emissions, even though they can comprise several technical units with different inputs and outputs. These highly aggregated results have little operational meaning and are unsuitable for comparison, especially since the interpretation of the accounting rules may differ from one site to another.[9] Moreover, the data can have large uncertainties and may not be mass balance consistent, which is not addressed by the current accounting methodology. This reduces the robustness of the accounting and increases the risk of not detecting errors coming from uncertainties or a poorly defined system (missing flows or stocks). Finally, the EU ETS only covers a limited number of GHGs and does not give credit for improving the end-of-life (EoL) management of waste flows (through better separation, reuse, or recycling).

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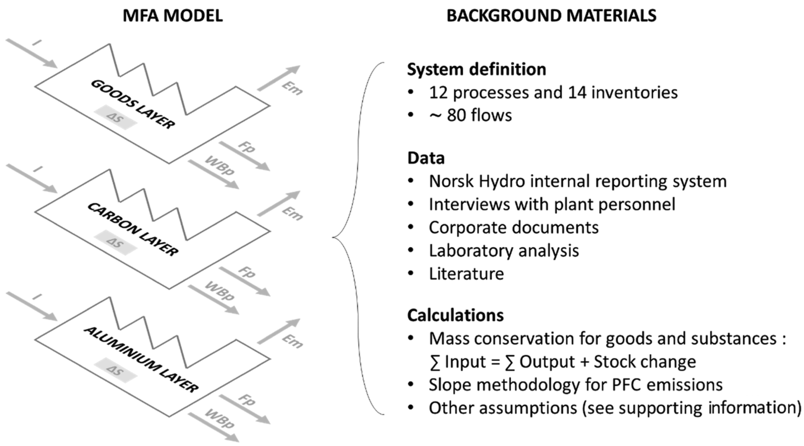

Figure 1. General principle for multilayer MFA model development. I = inputs; ΔS = stock change; Em = emissions; Fp = final products; WBp = waste and byproducts.

Tang and Luo[10] showed that companies with higher quality carbon management systems tend to achieve higher emission reductions but observed that carbon accounting and auditing alone had a limited effect, which they attributed among others to the lack of international standards. Indeed, because of the above-mentioned limitations, the EU ETS accounting is not the best tool to inform decision makers and plant managers about the performance of the sites. As a result, companies often develop and maintain separate accounting frameworks with an aim to inform mitigation strategies. However, these internal corporate accounting frameworks, although more refined, tend to neglect the systemic linkages between carbon emissions, materials, and energy. To understand causalities of emissions not only at the points where emissions occur but also emission changes caused throughout the system due to changes in material flows, carbon should be tracked (i) not only as emissions but throughout the system, in raw material inflows, intermediates, and byproducts, and (ii) not in isolation but understood as part of a complex system with feedbacks and delays. Climate change mitigation decisions based on attributional life cycle assessment frameworks and inventories might then lead to unintended systemic consequences.[11] In addition, these frameworks often list incomplete information[12] and are unsuitable for comparison between sites; hence, they are not suited to inform investors,[13] internal decision makers, and other stakeholders. Meanwhile, monitoring, reporting, and verifying emissions in the EU ETS represent an average yearly cost of 22 000 Euros per installation included. In relation to total emissions, these operational costs alone amount to 0.07 Euros per ton of carbon dioxide emitted[14] and stand for the greater part of the overall transaction costs associated with participating in the EU ETS.[14−16] However, despite such costs, there is still a lack of accounting tools that enable companies to identify and evaluate alternative strategies for saving resources and emissions.

Historically, material and energy balances at plant level have been used in steel production systems as part of the flowsheeting approach, originally developed for process optimization.[17−19] Porzio et al.[19] developed a decision support system for the steel industry based on flowsheeting, in which they modeled the main flows of products and materials within a plant and linked those flows with carbon dioxide emissions, enabling us to conduct forecasts and scenario analyses. While some early material flow analysis (MFA) studies had a plant-level focus,[20] this method has been mostly used as a tool to study global, national, or regional material cycles,[21] and very few plant-level MFAs have been performed so far. This is particularly the case for multilayer MFAs, which trace multiple individual chemical elements. The tracing of individual chemical elements is relevant for controlling the qualities of the main products, byproducts, and wastes or emissions. The optimization of the qualities of the different outputs, in turn, can have significant implications on the energy use and emissions. Plant-level MFA has recently regained attention, specifically to account for GHG emissions of steel production systems,[22,23] but those studies usually differentiate only one layer (total mass) and do not trace individual chemical elements/substances in designated layers. Some studies extended the spatial boundaries of the analysis beyond a single plant, such as Wu et al.[24] who analyzed the yearly exergy and energy flows as well as the carbon dioxide emissions of an iron and steel industrial network. Likewise, the scope has been extended to factory buildings, including, for instance, air conditioning and heating.[25,26] These approaches unveil greater potentials to reduce emissions, yet they differ with the perimeter commonly used to account for GHG emissions in the industry such as in the EU ETS guidelines. Gonzalez Hernandez et al.[27] used control data (i.e., with a very high temporal resolution) to quantify exergy flows and study resource efficiency in a steel plant. Their results gave operational details regarding the improvement measures that need to be implemented but are not linked with the yearly GHG emissions of the complete plant.

When it comes to aluminum, despite being one of the most studied metal cycles[28] at the global,[2,29,30] regional,[31] and country[32−37] levels, plant-level applications have been scarce. Hannula et al.[38] developed a simulation-based flowsheet for aluminum recycling and studied its resource efficiency through exergy analysis and life cycle assessment, but their system definition did not include a real-scale plant. While smelting is the most important process for both direct and indirect emissions in the aluminum cycle,[2] we could not find previous studies quantifying the entire metabolism of a primary aluminum plant nor did we find applications of MFA-based

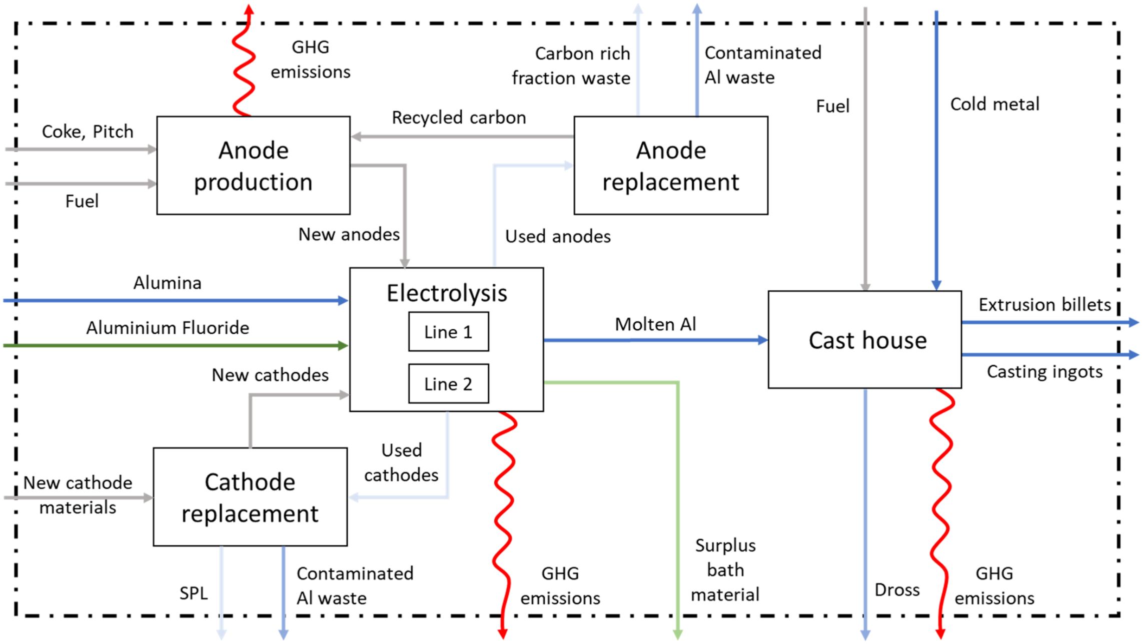

Figure 2. Simplified system definition of the plant. Aluminum-rich flows are shown in blue, carbon-rich flows in gray, fluorine-rich flows in green, and GHG emissions in red. Waste flows are shown in a lighter shade. SPL = spent potlining.

physical accounting for improving GHG emissions accounting, reporting, and mitigation.

Here, we perform a multilayer MFA to describe in a system context the metabolism of Norsk Hydro's primary aluminum smelter in Sunndal, Norway (the largest European smelter excl. Russia, with a design capacity of 300 + 100 kt Al/year in two smelting lines). We use this example to show how accounting tools that regard emissions as part of a larger production system can help to

(i) quantify GHG emissions of industrial facilities based on mass balance consistent physical accounting;
(ii) facilitate the identification of emission mitigation strategies to reach the EU ETS emission reduction targets—such as enhancing resource efficiency, substituting energy carriers, and improving specific processes; and
(iii) identify new levers to improve the sustainability performance of an industrial site by addressing systemic effects beyond the EU ETS scope.

METHODS

Plant-Level Multilayer Material Flow Analysis. We quantified the metabolism of the plant using the MFA methodology as described by Baccini and Brunner,[39] which tracks not only goods but also individual substances (a multilayer approach). Our system is quantified for three layers: goods, aluminum, and carbon. Figure 1 summarizes the general principle used in this study to perform the multilayer MFA. Stocks and flows of materials within the plant were quantified first for the goods layer. The aluminum and carbon layers were derived from the goods layer using concentrations of those two elements in the different goods. One of the basic principles of MFA is the conservation of mass, which holds for the three layers. This multilayer physical accounting allows us to better track the fate of individual chemical elements and improve the accuracy of the results by applying element-wise mass balance (Figure 2).

System Definition. The primary aluminum plant includes two smelting lines, a cast house, and three units dedicated to carbon anodes: one producing them, one rodding them to prepare them for smelting, and one cleaning the used anodes. The system was quantified for the three layers: goods, aluminum, and carbon. To be consistent with the EU ETS scope, the carbon layer covers the whole plant. The goods and the elemental aluminum layers are quantified for the whole plant with the exception of the cast house due to the complexity and limited data availability for the numerous flows of alloying elements.

The plant produces carbon anodes by mixing imported carbon-rich primary materials (tar pitch, petroleum coke) and recycled used anodes (so-called anode butts (AB)) into a paste. The anodes are subsequently shaped, baked, and then attached to a steel rod to be used in the smelting lines, where aluminum oxide is melted in a molten electrolytic bath. Aluminum fluoride and sodium carbonate are added for process control. Rodded carbon anodes are placed on top of the cells, and a carbon cathode is located at the bottom of the cell. While electric current goes from the anodes to the cathode through the molten bath, the carbon contained in the anodes binds with oxygen atoms in aluminum oxide and is emitted to the atmosphere (the Hall–Héroult process). The ideal theoretical reaction emits only CO_2, yet when the alumina concentration in the electrolytic bath is too low, a phenomenon called the anode effect (AE) occurs during which PFCs are emitted. Additionally, CO can be formed in the pots in a non-neglectable fraction due to the Boudouard

Table 1. Emission Reduction Estimation Method for Different Measures

measure	calculation for theoretical direct GHG emission reduction
improving alumina reduction (i.e., reaction occurring inside the pots during smelting)	difference between the calculated GHG produced in the anode gas and the theoretical GHG emissions from alumina reduction following the ideal reaction
reducing air burn	difference between the calculated GHG emissions in the exhaust gas from smelting and the calculated GHG emissions in the anode gas
diminishing AE	calculated PFCs emissions using the EU ETS slope methodology
limiting the amount of excess carbon (nonoxidized anodes) supplied to smelting	calculated assuming that all anodes were produced with the same carbon intensity as the one produced in the studied plant
reducing waste generation during anode production	assuming that the production of useful outputs of each process remains constant, that reducing waste generation allows us to decrease inputs and that the amount of fuel supplied is proportional to the total input of the process, we estimated GHG emission reduction potential for the anode paste plant, the anode baking furnace, and the anode rodding process
replacing liquid natural gas (LNG) in the anode plant and cast house with GHG-free energy carriers (hydrogen or electricity)	GHG emissions from LNG

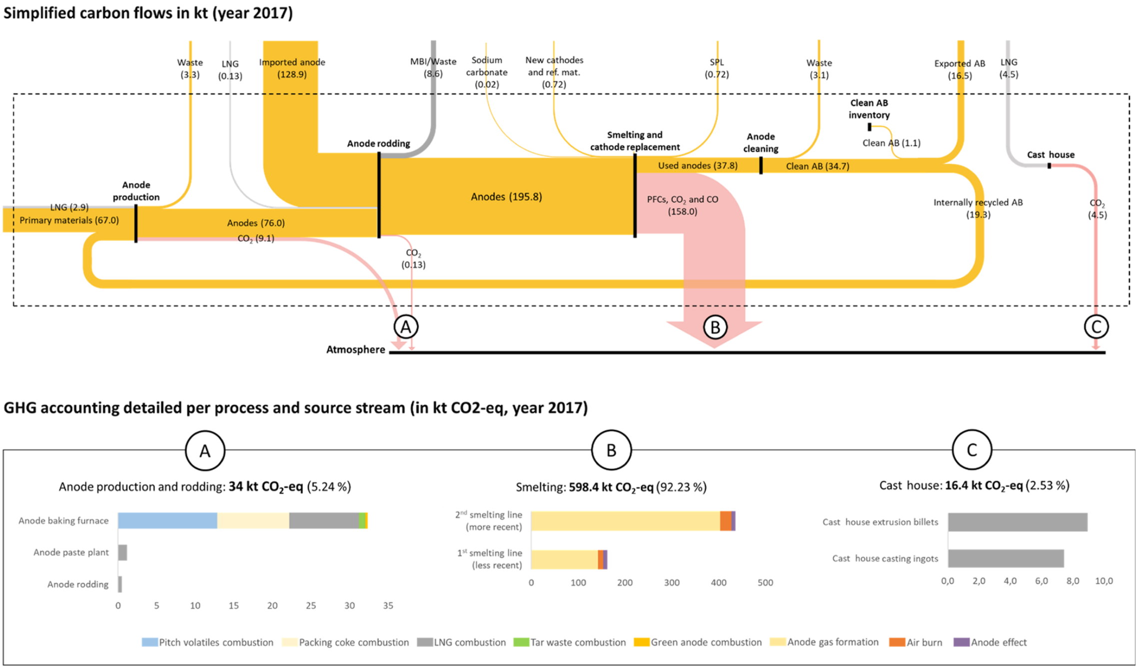

Figure 3. Simplified carbon flows (in kt of carbon) and associated GHG emissions (in kt CO_2-equiv) in 2017. Fuel flows are shown in light gray, mass balance inconsistency (MBI) in darker gray, GHG emissions flows in red, and other materials in yellow. MBI = mass balance inconsistency; AB = anode butts; PFCs = perfluorinated compounds; LNG = liquid natural gas; ref mat. = refractory materials; SPL = spent pot lining.

reaction[40,41] and the back reaction.[42] Although the carbon anodes are covered with anode cover material (ACM), a mixture of bath material (mostly composed of cryolite and chiolite) and alumina, part of it oxidizes with the ambient air.[40] The liquid aluminum resulting from this process sinks to the bottom of the cells, where it is tapped out daily. The molten aluminum is mixed with alloying elements and solid aluminum metal in the cast house to produce primary foundry alloys or extrusion billets.

The anodes have an average lifetime of 4 weeks, after which the remaining butts are removed from the pots and cleaned in several steps. This generates different waste flows that leave the plant for energy recovery or landfilling. The remaining clean carbon-rich fraction is recycled to make new anodes, either internally or externally. The average lifetime of a pot that contains the cathode is 4–6 years, after which pots are delined and relined with new refractory materials and a cathode. The waste from this process, called spent pot lining (SPL), is sorted into a contaminated carbon-rich fraction (first cut) and a contaminated, used refractory material fraction (second cut).

Quantification and Data Sources. All three layers were quantified for the year 2017. Inventories were introduced whenever necessary to capture relevant stock changes that might have occurred in the plant during the study year. Moreover, it was assumed that there was no stock change in the smelting lines (i.e., no stock change in the pots used to reduce alumina). The system was quantified using mostly internal reporting data. In cases of lacking or poor data, assumptions and estimates were made based on scientific literature, interviews with plant personnel, and corporate documents, or with the use of the mass balance principle. The carbon-containing exhaust gas from electrolysis was assumed to consist of CO_2, CO, and PFCs (Section S1). This assumption is consistent with the measured values in similar

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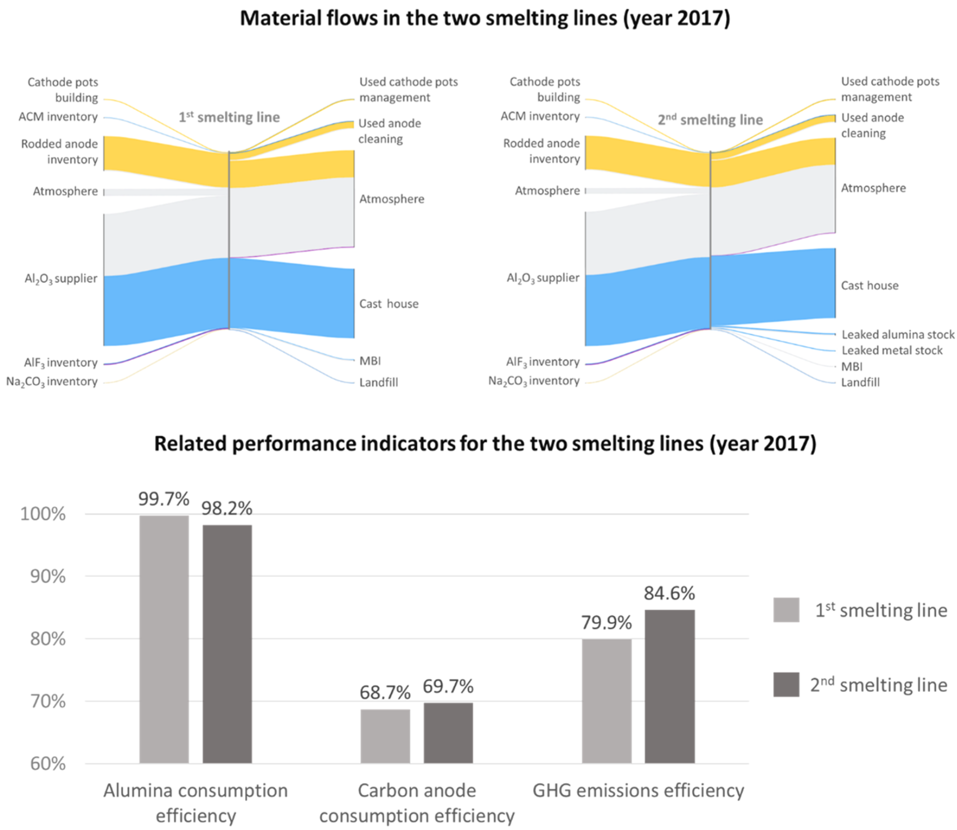

Figure 4. Example of detailed material flow analysis for the smelting processes and the related set of indicators. Upper part: aluminum flows are shown in blue, carbon flows in yellow, fluoride flows in purple, and other materials (mainly oxygen) in light gray. Internal recycling of Al_2O_3, AlF_3, and ACM within the smelting lines is not shown for reasons of simplicity; this choice of resolution does not affect the overall mass balance. A higher resolution might be useful for certain applications, including the development of additional indicators. MBI = mass balance inconsistency.

smelting lines[41] where other gases have proven to be present in negligible fractions. The ratio of CO_2 to CO emitted is assumed to be the same as the one measured by Kimmerle et al.[41] in a similar pot design, although CO emissions are neglected by the EU ETS methodology (Section S2.2). PFC emissions are calculated according to the slope methodology (Section S2.3) also used by the EU ETS[8] [Annex IV Section 8].

Potential for Emission Reduction. To illustrate the capabilities of the MFA approach, we used the system definition to identify the most promising technological measures to limit the overall plant-level emissions, making sure that the reduction in one process also minimizes the undesired impacts over the whole system. Table 1 lists those measures and shows how the potential emission reductions were calculated for the different intervention options. Detailed calculations are available in Section S3. All of these measures have been or are currently being considered by the aluminum industry, even if their implementation remains limited by uncertainties regarding economic profitability. The feasibility is not described further both for confidentiality reasons and because the main objective of this study is to demonstrate the potential of MFA for physical accounting, practical implementation of the reduction measures being out of the scope. The replacement of carbon anodes with inert anodes was not considered due to a lack of information about the implementation of this technology, including the feasibility of retrofitting of current smelting plants and potential trade-offs in energy use.[43] Besides, our current system definition would not be appropriate for a plant using inert anodes: entire subsystems like anode production and anode replacement would become obsolete, while new processes might need to be added, making a direct comparison difficult.

Uncertainties and Limitations. Norsk Hydro's internal reporting system provided reliable data to quantify most material flows. Nevertheless, some parts of the system were quantified using assumptions with a relatively high uncertainty, such as for the flows related to SPL production or the ratio of CO_2 to CO emitted to the atmosphere. A qualitative analysis of the level of uncertainty of the main parameters and assumptions as well as quantification methods for the different flows is presented in Sections S4 and S5, Supporting Information.

To understand the potential influence on the results of the most uncertain parameters, a one-factor-at-a-time sensitivity analysis was conducted on the main GHG emission flows (emissions from the smelting lines and the anode baking

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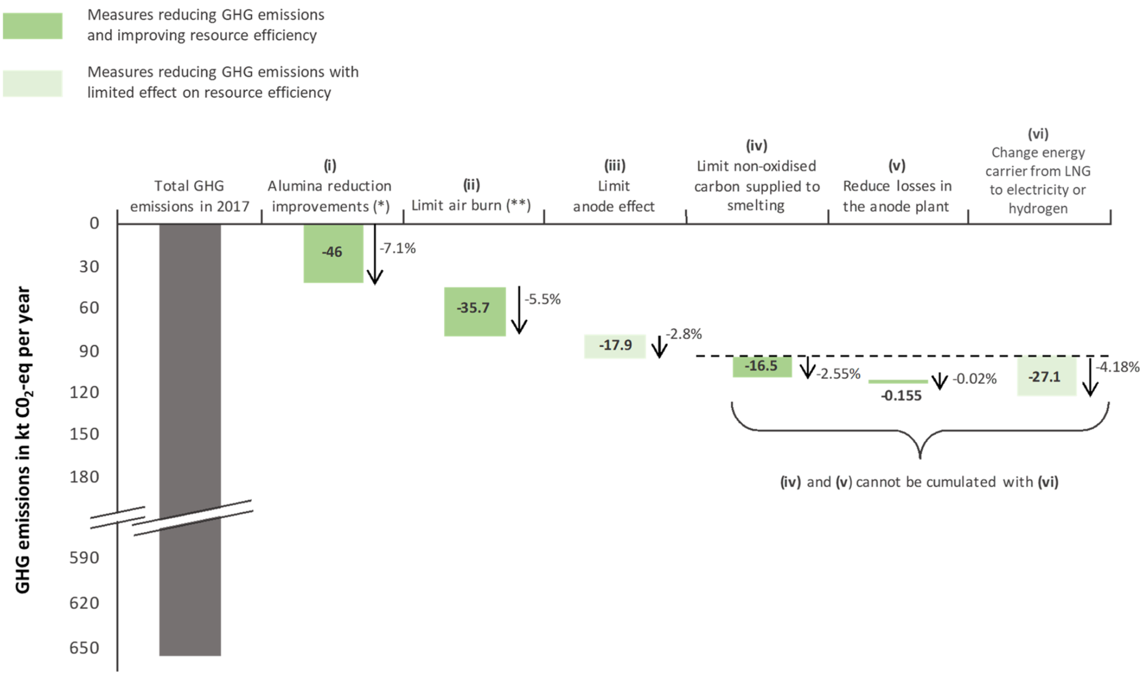

Figure 5. Theoretical yearly GHG emission reduction potential. (*) Alumina reduction improvements refer to increasing the proportion of carbon reacting ideally during smelting and limiting CO_2 burn and back reaction. (**) Decrease in the amount of carbon oxidized via air burn during smelting and oxidation of carbon monoxide from the exhaust gas with ambient air. LNG = liquid natural gas.

furnace). A description of the methodology and detailed results are presented in Sections S6 and S7.

■ RESULTS

Carbon Layer and GHG Emissions. Figure 3 presents simplified results of the carbon layer MFA and detailed GHG emissions accounting for the year 2017, obtained by systematically tracking carbon flows within the plant. Results are consistent with the existing literature and previous measurements, such as the emission intensity of the smelting process[44] and its excess carbon consumption,[42] CO_2 to CO ratio in the anode gas from smelting,[45] and weight loss of the anodes during the baking process.[44] Detailed Sankey diagrams of the anode plant and anode cleaning subsystems are available in Sections S8 and S9.

System-Based Indicators. As illustrated here for the two smelting lines of the plant, our approach enables the design of a set of system-based indicators that integrates both resource efficiency and GHG emission levels. Figure 4 shows that the second smelting line operates closer to the theoretical optimum (see Section S10) when it comes to GHG emissions and carbon consumption. Looking at aluminum extraction from alumina, the first smelting line performs slightly better than the second one. This is due to spillage in the second smelting line, as shown in the Sankey diagram of Figure 4. The real efficiency of the reduction process occurring inside the pots of the second smelting line is hidden by the spill: if it were plugged, all things being equal, it would perform better than the first line.

Theoretical Emission Reduction Potential of Technological Mitigation Options. Figure 5 shows the theoretical potential of different options to reduce the yearly GHG emissions of the studied plant. The greatest emission reduction potential lies in improving the smelting process (−116 kt CO_2-equiv, i.e., 18% decrease compared with 2017 levels).

Improving alumina reduction so that the cells can operate closer to the theoretical reaction had the potential to reduce annual emissions by 7.1% in 2017. Nevertheless, this will be challenging from a technical point of view: the plant studied consumed less than 0.4 kg of carbon per kg of aluminum produced, one of the lowest values reported in the industry.[44,46] The net carbon consumption could be reduced by increasing the pitch content of the anodes,[47] given that locally produced anodes contain 13.3% of pitch, while this value ranges from 13 to 18% in the industry.[44] Additionally, net carbon consumption could be reduced by decreasing the metallic impurity content in the anodes.[47] This would require improved waste sorting technologies, as we estimated that carbon anode butts recycled in the plant in 2017 contained 1.18% of aluminum impurities after going through the cleaning processes.

Reducing air burn, for example, by covering the upper part of the anodes more carefully to limit contact with oxygen from the ambient air,[40,48,49] has a great potential to cut direct emissions (−5.5% in 2017). Since it has little influence on the bath chemistry, it might prove easier to implement than improving alumina reduction. Increasing the thickness of the anode cover material (ACM), novel coating techniques, and other technologies could further help to meet this ambition.[48−50]

Industry has focused a lot on reducing AE in the past few decades;[51] consequently, results showed that reducing it

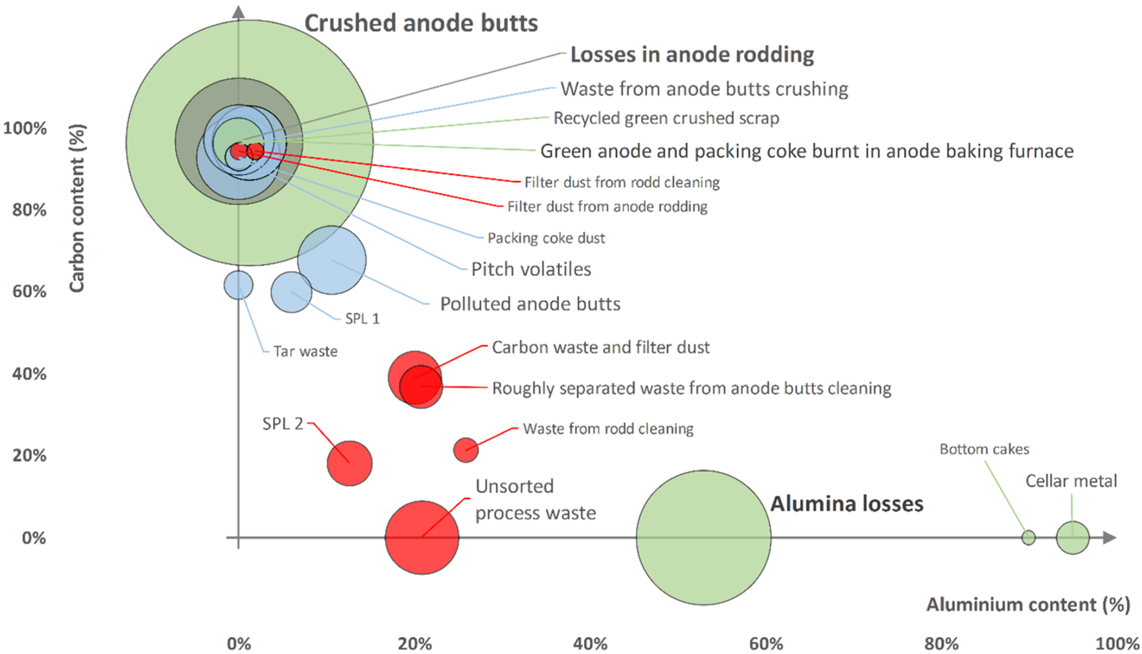

Figure 6. Overview of the different waste flows generated in 2017 according to their Al and C content and their EoL management method. SPL1 = spent potlining first cut, i.e., carbon fraction; SPL2 = spent potlining second cut, i.e., refractory fraction. Color of the dots refers to their EoL management method: green = recycled, blue = energy recovery, red = landfilled. Size of the dots refers to the weight of the waste stream (the bigger dot being 33.5 kt and the smaller 0.4 kt).

further would have a lower impact than the measures mentioned above to reduce direct GHG emissions. Reducing AE can be achieved by improving computer control of the operating procedures,[52] but it might be challenging with the current cell technology because the performance of the plant is very close to the industry's best practice reported by Cusano et al.[44] The reduction potential would however be much higher for older or less performant plants.

Waste reduction in the anode plant could cut annual direct emissions by 0.02% (155 kg CO_2-equiv/year), while changing the energy carrier from LNG to hydrogen or electricity would result in a reduction of 4.18%/year. However, even if the hydrogen option is currently being considered,[53] the technical feasibility is still uncertain, and benefits would need to be evaluated in a broader system considering electricity/hydrogen production and transport.

Streams of Waste and Byproducts. Figure 6 shows an overview of the waste streams, their composition (Al and C content), and EoL treatment. We identified clusters of waste/byproducts depending on their composition, which often determines their preferred EoL treatment: (i) the waste containing almost pure carbon is internally recycled, (ii) the waste with a high carbon content (60–70%) and a low aluminum content is used for energy recovery, (iii) the waste containing significant fractions of both carbon and aluminum is landfilled, and (iv) the waste with a high aluminum content and a very low carbon content is externally recycled. This synthesis enables a first crude evaluation of the EoL treatment options for different waste streams. For instance, not all waste flows from the cluster (i) are recycled: although they share the same characteristics in terms of composition, some are used for energy recovery or even landfilled. Similarly, one could investigate to which extent the waste used for energy recovery outside the plant could be used locally as a substitute for imported fuel, thereby decreasing indirect GHG emissions and costs associated with transportation.

DISCUSSION

Increase the Robustness and Relevance of GHG Reporting with MFA-Based Accounting. Plant-level MFA enabled the quantification of GHG emissions with a greater level of detail than the EU ETS accounting methodology, shedding light on emissions from each process and breaking down the emissions per source reaction. Compared with the MFA-based GHG accounting, the EU ETS slightly overestimates the total GHG emissions (+4.2%), yet it is difficult to allocate this difference to a specific cause due to the low level of detail provided by the EU ETS accounting. The sensitivity analysis suggests that results are robust for GHG emissions as the most uncertain parameters, including the ratio of CO_2 to CO in the exhaust gas, have no or very little influence on these flows (Section S7). Hence, neglecting CO emissions from smelting—as done in the EU ETS accounting—seems reasonable to evaluate the total bulk GHG emissions of the plant. Nevertheless, taking CO emissions into account using an MFA-based methodology provides further insights into the causes of the emissions, such as distinguishing between alumina-based anode oxidation and air burn.

Like the EU ETS methodology, our physical accounting approach only considers direct GHG emissions of industrial sites. However, the better understanding of linkages between

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emissions and material flows is a good starting point for the inclusion of scope 2 and 3 emission inventories, which is needed to avoid problem shifting and design more ambitious strategies. Our study differentiates only two elemental layers, carbon and aluminum, which is sufficient to illustrate the main systemic effects between resource use and GHG emissions. However, additional linkages could be uncovered by considering additional chemical elements, such as fluorine and sodium. Similarly, adding energy and/or exergy layers would allow potential trade-offs between material and energy efficiency to be better quantified.

While the EU ETS methodology only considers aggregate stock changes at the plant level and does not differentiate inventory changes in different parts of the system, MFA-based accounting includes inventories in a more detailed and consistent way. This allows us to explicitly consider the time lag between emissions in different parts of the system and the sales/production, which is better aligned with reality and therefore better suited for tracking performance over time. An illustration is that following the EU ETS methodology, traded quantities of waste are used as a proxy to quantify produced quantities. For instance, inventories of clean anode butts (Figure 3) are often neglected; hence, emission calculation differs from the actual production activity.

MFA-based accounting is also more robust because it enables mass balance consistency checks and facilitates the identification of inconsistencies in different parts of the system. Based on the data available to perform the MFA, the anode rodding process of the plant held a mass balance inconsistency of 8.6 kt of carbon in 2017 (i.e., 8.6 kt of carbon were missing from the outflow of this process). The EU ETS methodology would not enable us to spot this inconsistency and would account for missing outflows from the carbon balance of the plant as emission flows by default—standing for 31.5 kt CO_2 in the case of the inconsistency mentioned above. On the contrary, further investigations showed that the inconsistency was due to data uncertainty and/or unaccounted solid waste. Ensuring that the material balance of the plant is respected through data reconciliation—made especially possible here by performing a multilayer MFA—reduces the uncertainty of the results. Some of the mass balance inconsistencies may also be attributed to the time resolution chosen. The annual balance applied here is usually sufficient to balance out short-time fluctuations, although some inventories change over longer periods, requiring either a longer balancing period or a higher time resolution for stock accumulation and depletion.

Reconcile EU ETS and Internal Reporting. The EU ETS methodology is a robust framework to quantify bulk GHG emissions within a reasonable margin of error, while physical accounting provides deeper insights into sources and causes of emissions. The MFA-based tool builds on existing plant-level data to link physical accounting and carbon reporting. Increased granularity and consistency between materials and emission inventories enable us to use the same data to produce the EU ETS reporting and the set of system-based indicators that is used internally to manage performance improvement.

Identify and Assess Systemic Emission and Resource Efficiency Strategies. Maps of a plant's material and energy stocks and flows (metabolism), combined with scenario analysis tools, can help plant managers to identify not only conventional options for direct emissions saving in isolated processes but also systemic solutions considering linkages between emissions, materials, and energy in different processes and at the plant level. For instance, the aluminum industry has historically focused on reducing AE due to direct productivity and environmental benefits, but our results show that there might be a greater potential in the future for reducing air burn and the amount of nonoxidised carbon supplied to the smelters. Additional emission reduction potentials could be identified with extended system boundaries, for example with a better separation of the different material layers in the cast house or by the inclusion of energy flows. While traditional mitigation options have relied on conventional process-oriented areas of research, which tend to focus on processes where emissions and costs are the highest (e.g., electrolysis), the analysis of a plant's metabolism can shed light on systemic strategies for emission reduction, an area that is vastly underexplored.

Applying MFA at the plant level also enables the investigation of potentials for improvements beyond the boundaries of the EU ETS GHG accounting, such as reducing indirect GHG emissions and improving resource efficiency via alternative waste and byproducts management (e.g., alumina losses into the basement of the smelter as shown in Figure 6). It highlights issues left out by the EU ETS accounting, which considers all exported carbon-containing waste as carbon stored without introducing any concept of responsibility for the waste producers, making it easier to shift the waste-handling burden downstream in the production line. One could argue that resource efficiency and waste management are out of the scope of the EU ETS accounting, yet research showed that these topics are intrinsically connected with GHG emission mitigation.[54] For instance, Figure 5 shows that reducing the amount of anode nonoxidized during smelting has the potential to reduce annual emissions in the production phase of the anodes by 16.5 kt CO_2-equiv, which stands for 2.55% of the direct emissions in 2017.

Physical accounting at the plant level not only unveils potentials to reduce GHG emissions but regards emissions as part of a larger production system. It enables us to investigate the resource efficiency improvements, for instance, via alternative waste and byproducts management, which are not captured by the EU ETS framework. Thereby, it informs long-term strategies for industries to meet the EU ETS targets and reduce yearly emissions.

Save Costs. GHG accounting is often considered an important cost factor for companies. However, if the accounting tool used has multiple functions and can help identify the most effective options for saving resources and emissions, the accounting tool may also result in cost savings. Hence, the use of plant-level MFA by corporate decision makers might increase the attention put into GHG emission accounting and mitigation by unveiling synergies with resource efficiency improvements. Above, we proposed four (out of six) theoretical emission reduction measures that would also decrease raw material consumption. Our approach also helps industries to meet the emission reduction targets and to lower the costs of emission taxes.

Conclusion: Implications of Using Physical Accounting in Industrial Sites. While emission reporting and resource efficiency are traditionally analyzed in different systems within a given industrial site, we integrated them in a single framework by studying the plant's metabolism and systematically tracking resource and emission flows. We built a tool consistent with the internal reporting system of the

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company so that once established it can easily be updated and adapted to the needs of plant managers.

Physical accounting based on plant-level MFA has the potential to inform long-term investment strategies for resource efficiency and GHG emission reduction targets to link these strategies with operational management and accounting tools and, in fine, to reach the emission reduction targets set by the EU ETS. If applied widely in industry, this approach opens up the prospect of faster, deeper, and cheaper improvements in resource efficiency and climate change mitigation.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acs.est.1c05681.

Methodology for calculation of emission flows; list of assumptions used to quantify the system; EU ETS framework methodologies; theoretical emission reduction potential calculations; list of assumptions used to quantify the system; quantification methods for the different layers and flows of the system; sensitivity analysis methodology and results; detailed Sankey diagrams of the anode plant and anode cleaning subsystems; performance indicator calculations (PDF)

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Author Contributions

R.G.B., D.B.M., and E.N. designed the study; L.M., E.N., and M.I. collected the data; L.M. conducted the analysis, with help from R.G.B., E.N., and D.B.M.; R.G.B. and L.M. led the writing of the paper; all authors interpreted the results, reviewed the paper, and approved the final version of the manuscript.

Notes

The authors declare no competing financial interest.

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Paper 3

A GENERAL FRAMEWORK FOR STOCK DYNAMICS OF POPULATIONS AND BUILT AND NATURAL ENVIRONMENTS

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A general framework for stock dynamics of populations and built and natural environments

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Abstract

Sustainable development involves a responsible management of the interactions between humans and their built and natural environment. From a physical perspective, the interactions can be characterized as stocks and flows of energy and matter within and between these spheres. Understanding the dynamics of the stocks is essential to enable their responsible management. A large number of independent disciplines study the dynamics of individual stocks with specific methods. The resulting fragmentation of methods hampers interdisciplinary learning, including the integration of more specialized discipline-specific models into more encompassing ones. Here, we develop a general mathematical framework for dynamic stock models based on balance, intrinsic, and model-approach equations. We use the framework to classify a variety of stock models from different disciplines and discuss their applicability. The framework provides a common language for the interdisciplinary analysis of coupled human–environment systems. This article met the requirements for a gold-gold *JIE* data openness badge described at http://jie.click/badges.

KEYWORDS
demographic metabolism, industrial ecology, material and energy flow analysis, population dynamics, socio-economic metabolism, stock dynamics

1 | INTRODUCTION

Sustainable development, from a physical perspective, is all about a conscious exchange of matter and energy between human societies and their built and natural environment. Mankind has always shaped the built environment in order to meet its needs for food, shelter, work, transport, communication, and cleaning (Baccini & Brunner, 1991, 2012) and thereby also altered the natural environment. However, technological progress has enabled human populations to grow to unprecedented levels and to transform the built and natural environment at extraordinary rates (Crutzen, 2002). Most of the United Nations' Sustainable Development Goals (SDGs) (United Nations General Assembly, 2015) are directly linked to these transformations, including SDG1 (no poverty), SDG2 (zero hunger), SDG6 (clean water and sanitation), SDG7 (affordable and clean energy), SDG8 (decent work and economic growth), SDG9 (industry, innovation, and infrastructure), SDG11 (sustainable cities and communities), SDG12 (responsible consumption and production), SDG13 (climate action), SDG14 (life below water), and SDG15 (life on land).

In fact, Griggs et al. (2013) advocated for SDGs focusing on both poverty reduction and protection of the Earth's life support system as opposed to the Millennium Development Goals, which focused heavily on poverty reduction. They support their advocacy with the concept of a "*safe* *operating space for humanity"* defined by "*planetary boundaries"* (O'Neill et al., 2018; Rockström et al., 2009; Steffen et al., 2015) that correspond to limits on concentrations of problematic substances in certain environmental reservoirs, such as the atmosphere and the oceans. The actual concentrations depend on the biogeochemical and anthropogenic cycles of the respective elements (Chen & Graedel, 2012a). These cycles link the human population with reservoirs in the built and natural environment through exchanges of matter and energy over time (Haberl et al., 2019). It is therefore essential to develop an understanding of the concurrent dynamics of the human population as well as the built and the natural environment (Krausmann et al., 2017; Lutz, 2017; Müller et al., 2013; Pauliuk & Müller, 2014; Weisz et al., 2015). Here, we understand the built environment to encompass all physical stocks amassed by human societies except for human bodies, livestock, and crops (Bartuska, 2007). This notion is also known as "*technomass*" (Inostroza, 2014), *"manufactured capital"* (Weisz et al., 2015), or "*material stocks"* (Haberl et al., 2019).

Several disciplines analyze the stocks and flows of anthropogenic and natural systems, including demography (Lutz, 2012), epidemiology (Schoenbach, 2007), population ecology (Beddington & May, 1977; Anderson et al., 2008), industrial ecology (Frosch, 1992), economics (Cleveland et al., 1984; Costanza et al., 1997), urban planning (Wolman, 1965; Inostroza, 2014), engineering (Allwood et al., 2011), and forestry (Müller et al., 2004). These disciplines have often developed their own languages and tools for analyzing stock dynamics in sophisticated ways within their systems of interest. This fragmentation in languages and tools hampers a common learning process as well as the integration of anthropogenic and natural systems into more comprehensive models (Haberl et al., 2019). Integrated assessment models, for example, have only recently started to include built environment stocks explicitly (Pauliuk et al., 2017), and are in the process of refining the resolution of population stocks (Samir & Lutz, 2017). Vásquez Correa (2018) has begun to model both the demographic (Lutz, 2012) and the socio-economic (Fischer-Kowalski & Haberl, 1998) metabolism to study food and housing demand.

To facilitate the development of such models in the future, we (i) develop a general framework for dynamic stock models, (ii) use this framework to classify different ways of describing dynamic stock models, and (iii) discuss how our framework can be applied to human populations and to stocks in the built and natural environment. Our focus lies on physical systems of stock and flow relationships that are common to all three domains, while omitting the exploration of domain-specific external drivers.

Notation. Vectors are denoted by uppercase letters in boldface.

2 | FRAMEWORK DEVELOPMENT

2.1 | Conservation principles and system variables

The terminology of material flow analysis (MFA) set forth by Baccini and Brunner (1991), Baccini and Bader (1996), as well as Brunner and Rechberger (2004) builds on the notion of mass conservation and defines *processes* as spatially defined balance volumes that include a "*transport, transformation, or storage"* of materials. MFA has since been extended to include energy balances (Müller et al., 2004) and been used to measure national and global material stocks and flows (Fischer-Kowalski et al., 2011; Schandl et al., 2018; Wiedenhofer et al., 2019).

Here, we expand the notion of processes to balance volumes of any physical entity, including humans, animals, plants, or man-made artefacts. The expansion needs to be dealt with carefully. The first law of thermodynamics states that energy can neither be created nor destroyed. In the absence of nuclear reactions, it implies the principle of mass conservation. Entities such as living organisms and man-made artefacts, however, undergo cycles of creation and destruction, and obey conservation principles only within further limitations. The conservation of entities other than energy or mass is nevertheless useful in many applications, provided that these limitations are carefully considered by treating creation and destruction as in- and outflows. Demography, for example, accounts for births and deaths to balance human populations (Land et al., 2005).

In MFA, *stocks* are traditionally defined as quantities of mass or energy in spatially delimited balance volumes at specific points in time. Other entities are included in MFA either as carriers (called goods) of materials and energy or as exogenous parameters influencing mass and energy flows and accumulations. For example, Müller (2006) calculated the quantity of concrete in the Dutch dwelling stock as a function of the Dutch population and its housing needs.

Here, we define *stocks* as quantities of general entities in processes. *Flows* represent the amount of entities exchanged between two processes in a fixed period of time. The temporal evolution of a process over a time horizon T can therefore be described by its stock, S, its inflows, I, and its outflows, O. Consistent with MFA terminology, we refer to these variables collectively as *system variables*. The time horizon is often discretized into $N = T/\Delta t$ periods of length Δt. We denote the stock at the *end* of period t by S_t and the inflow and outflow *during* period t by I_t and O_t, respectively. The system variables are then time series, which we henceforth represent mathematically by the non-negative N-dimensional real row vectors $\boldsymbol{I}$ and $\boldsymbol{O}$ for I and O, respectively, and the non-negative $(N+1)$-dimensional real row vector $\boldsymbol{S}$ for S.

The conservation principles imply that any difference between the in- and outflow during any period t translates into an equal difference between the stock at the end and the beginning of period t. Formally, the stock change, ΔS_t, during any period t obeys the *balance* (Equation 1) and the *intrinsic* (Equation 2) equation.

$$\Delta S_t = I_t - O_t \tag{1}$$
$$= S_t - S_{t-1} \tag{2}$$

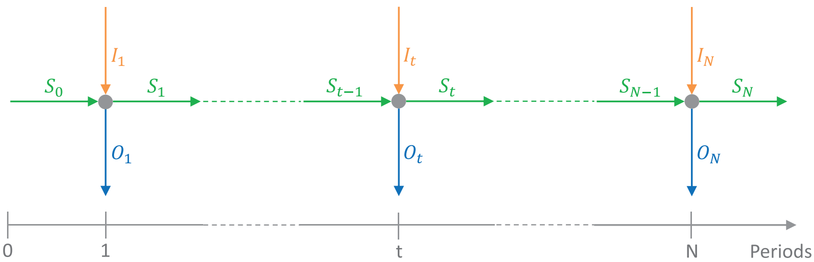

FIGURE 1 Network representation of a dynamic stock model

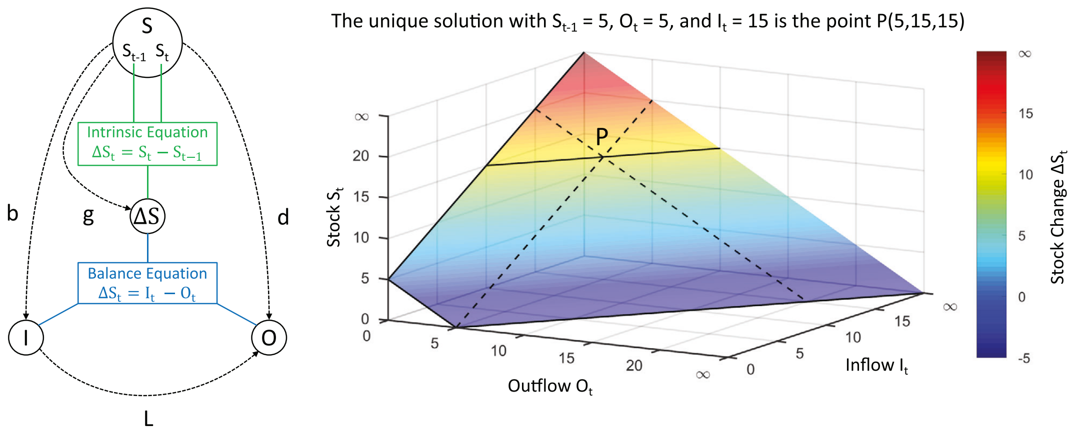

FIGURE 2 Left: The balance and intrinsic equations link the stock, *S*, with the inflow, *I*, and the outflow, *O*. Model-approach equations link the system variables through birth, *b*, death, *d*, or growth, *g*, rates or lifetimes, *L*. Right: The balance, the intrinsic, and one model-approach equation define a plane on which the other two model-approach equations define a point (visualized here for three dimensions)

Note that as opposed to the system variables, the stock change may adopt both positive and negative values.

One can visualize the conservation principles by representing the system variables as flows in a directed graph, whose arcs correspond to components of the system variables ***I***, ***O***, and ***S***, and whose nodes correspond to the periods $t = 1, \ldots, N$ (Figure 1). Note that the term "*flow*" in graph theory does not only refer to physical flows as in MFA, but can refer to any system variable, including physical stocks. In graph theory terminology, the conservation principles translate into *flow conservation*, meaning that the total flow entering a node equals the total flow exiting that node, either as an outflow or stock change.

The evolution of the system during any period *t* is described by the five *analysis variables* (I_t, O_t, ΔS_t, S_{t-1}, S_t), where S_{t-1} plays the role of an initial condition. Although not strictly needed, we added the stock change during period *t* to the list of descriptors for ease of analysis. The variables may be calculated with the help of five linearly independent equations, which are the balance and intrinsic equations (Equations 1 and 2) and three additional *model-approach equations*.

2.2 | Model-approach equations

Model-approach equations consist of parameter functions that are not necessarily founded in physical laws. They often depend on the purpose of the model and are estimated from expert judgement, empirical evidence, or physical models. Forest succession models, for example, may estimate birth, death, and growth rates based on a variety of environmental factors such as temperature, soil humidity, and light availability (Larocque et al., 2016). In general, model-approach equations either define an analysis variable directly, for example, by defining an individual flow or an initial condition for the stock, or link two analysis variables (Figure 2). For instance, they may link:

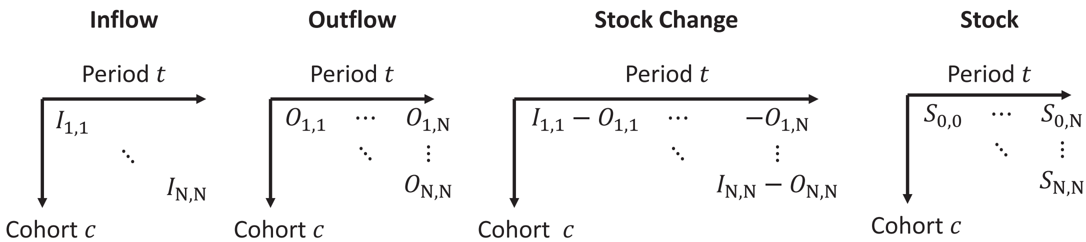

FIGURE 3 Matrix description of the analysis variables' cohort composition over *N* periods

1. Inflow and outflow. The relation between in- and outflow is determined by a time delay, which is often referred to as the *lifetime*, *L*. For living organisms, lifetime is a trivial concept. For non-living entities however, the terms "*delay*" or "*residence time*" might be more appropriate. Here, we use the term "*lifetime*" because it is common in many disciplines.
2. Inflow and stock. In population dynamics, the relation between inflow and stock is termed *birth rate*, *b*. It relates the stock at the end of the previous period to the inflow during the current period. Birth rates for physical goods are often called differently, such as "*construction rates*" for buildings. For the sake of simplicity, we henceforth use the term "*birth rate*" for both living organisms and physical goods.
3. Outflow and stock. In demographics, the relation between the stock at the end of the previous period and the outflow during the current period is known as *death rate*, *d*. Death rates correspond to leaching rates (van der Voet et al., 2002) for the loss of materials or substances.
4. Stock and stock change. *Growth rates*, *g*, relate the stock at the end of the previous period with the stock change during the current period.

More elaborate model-approach equations may rely on several parameters to relate more than two system variables with each other. For example in demography, the Gompertz–Makeham law of mortality (Makeham, 1860; Missov & Lenart, 2013) stipulates that the outflow O_t during period t of an inflow I_{t_0} during period t_0 is the sum of a term, $\alpha e^{\beta(t-t_0)} I_{t_0}$, that increases exponentially with age, $t - t_0$, (which corresponds to a lifetime function), and a term, λS_{t-1}, that depends on the stock size only (which corresponds to a death rate).

In general, the parameter values can change over time. For instance, human life expectancy has increased dramatically over the last 200 years (Horiuchi, 2000). Keeping track of the period in which entities are created, that is, their *cohort*, will allow us to consider time-dependent parameters explicitly, for example, by assigning a different lifetime to each cohort.

2.3 | Cohorts

In general, the analysis variables may contain elements of the cohorts $c = 1, \ldots, t$ for any period t. Their cohort composition can be represented by upper triangular matrices whose rows and columns correspond to cohorts and time periods, respectively. For example, $O_{1,2}$ is the outflow from cohort 1 during period 2. Here, we focus on new inflows with age zero, that is, on diagonal inflow matrices (Figure 3). If we allowed for inflows of old cohorts (e.g., imports of used goods or immigration), then the inflow matrix would also be upper triangular.

The balance and intrinsic equations apply to each cohort c individually. In combination with the non-negativity of the inflow, outflow, and stock, they imply that for any period t the sum over the outflows of cohort c that have occurred up to period t must be smaller or equal to the inflow of cohort c

$$\sum_{\tau=1}^{t} O_{c,\tau} = \sum_{\tau=c}^{t} O_{c,\tau} \leq I_{c,c} \tag{3}$$

and that for any cohort c between 1 and t, the quantity of cohort c in the stock at the end of period t is given by the inflow during period c minus the outflows of cohort c during the periods $c, \ldots, t$.

$$S_{c,t} = I_{c,c} - \sum_{\tau=c}^{t} O_{c,\tau} \tag{4}$$

In general, the initial stock may be non-zero, in which case it consists of cohorts predating the beginning of the modeling time horizon. For Equation (4) to be well defined for all cohorts from the oldest cohort in the initial stock to the youngest cohort in the terminal stock, one may artificially prolong the modeling horizon into the past, so as to include the inflow of the oldest cohort in the initial stock. The stock of all cohorts that matter for the original horizon will then be zero at the beginning of the prolonged horizon and can be described by Equation (4). This will enable us to derive several more equations governing stock dynamics. The price of the horizon extension is an increase in the dimension of all analysis variables and all parameters. As the extended model considers only flows of cohorts that are relevant for the original horizon, it does not properly describe the state of the system before the beginning of that horizon.

The concept of cohorts enables us to define a *lifetime matrix*, L, whose component $L_{c,t} = O_{c,t}/I_{c,c}$ is the fraction of $I_{c,c}$ that leaves the stock during period t. After extending the time horizon, we can assume that the number of cohorts equals the number of time periods. This implies that the lifetime matrix is square and as such may be invertible.

$$L = \begin{bmatrix} O_{1,1}/I_{1,1} & \cdots & O_{1,N}/I_{1,1} \\ \vdots & \ddots & \vdots \\ 0 & \cdots & O_{N,N}/I_{N,N} \end{bmatrix} \quad (5)$$

The lifetime matrix yields an easy way to calculate the aggregated outflow $O_t = \sum_{c=1}^{t} O_{c,t}$ during period t as a function of the inflows during the periods $1, \ldots, t$. To see this, denote the aggregated in- and outflow and the stock change from all cohorts during the periods $1, \ldots, N$ as row vectors $\boldsymbol{I} = (I_1, \ldots, I_N)$, $\boldsymbol{O} = (O_1, \ldots, O_N)$, and $\boldsymbol{\Delta S} = (\Delta S_1, \ldots, \Delta S_N)$, respectively. The aggregated outflow during any period t is $\sum_{c=1}^{t} I_c L_{c,t}$ which corresponds to the scalar product between the inflow vector $\boldsymbol{I}$ and the t^{th} column of the lifetime matrix L. Therefore, the aggregated outflow vector $\boldsymbol{O}$ is given by the matrix product between $\boldsymbol{I}$ and L

$$\boldsymbol{O} = \boldsymbol{I}L, \quad (6)$$

which allows us to express the stock change as a function of $\boldsymbol{I}$ and L,

$$\boldsymbol{\Delta S} = \boldsymbol{I} - \boldsymbol{O} = \boldsymbol{I} - \boldsymbol{I}L = \boldsymbol{I}(\mathbb{I} - L), \quad (7)$$

where $\mathbb{I}$ is the identity matrix of size N. The inflow can now be expressed as a function of the stock change and the lifetime,

$$\boldsymbol{I} = \boldsymbol{\Delta S}\,(\mathbb{I} - L)^{-1}, \quad (8)$$

if and only if $(\mathbb{I} - L)$ has full rank, that is, all its diagonal elements are greater than zero. This is the case if and only if the time resolution of the model is fine enough to ensure that no cohort enters and completely leaves the stock during one and the same period.

Recall that the stock change can be computed via the intrinsic equation if the evolution of the stock is known. Equation (8) may thus be used in *stock-lifetime-driven* models to determine inflows given the lifetime matrix and the evolution of the stock. Solving the equation may seem somewhat cumbersome because it involves the inverse of the matrix $(\mathbb{I} - L)$. As this matrix is upper triangular, however, the equation can be solved by forward substitution (Horn & Johnson, 1985; Hackbusch, 2015), that is, by subsequently calculating the inflow during all periods. Doing so takes at most $N(N+1)$ arithmetic operations. This means that solving stock-lifetime-driven models only takes N more arithmetic operations than solving *inflow-lifetime-driven* models, where outflows are calculated by the matrix product of inflows with the lifetime matrix. If the stock's cohort composition is known, the inflow of a specific cohort c can even be found directly by examining the stock of cohort c at the end of a period $t \geq c$ such that $S_{c,t} > 0$. In fact, Equation (4) yields

$$S_{c,t} = I_{c,c} - \sum_{\tau=c}^{t} I_{c,c}\,L_{c,\tau} = I_{c,c}\left(1 - \sum_{\tau=c}^{t} L_{c,\tau}\right) \Leftrightarrow I_{c,c} = \frac{S_{c,t}}{1 - \sum_{\tau=c}^{t} L_{c,\tau}}. \quad (9)$$

While the balance and the intrinsic equations are common to all dynamic stock models, the model-approach equations depend on the purpose of the model and on the available prior information about the system variables. Therefore, different disciplines may be familiar with different model-approach equations. In the next section, we provide a table that classifies dynamic stock models based on the model-approach equations and the prior information they assume.

3 | CLASSIFICATION OF DYNAMIC STOCK MODELS

Figure 4 shows 21 combinations of model-approach equations with prior information about system variables. Each of these combinations allows for the direct determination of the unknown system variables and is therefore a valid dynamic stock model.

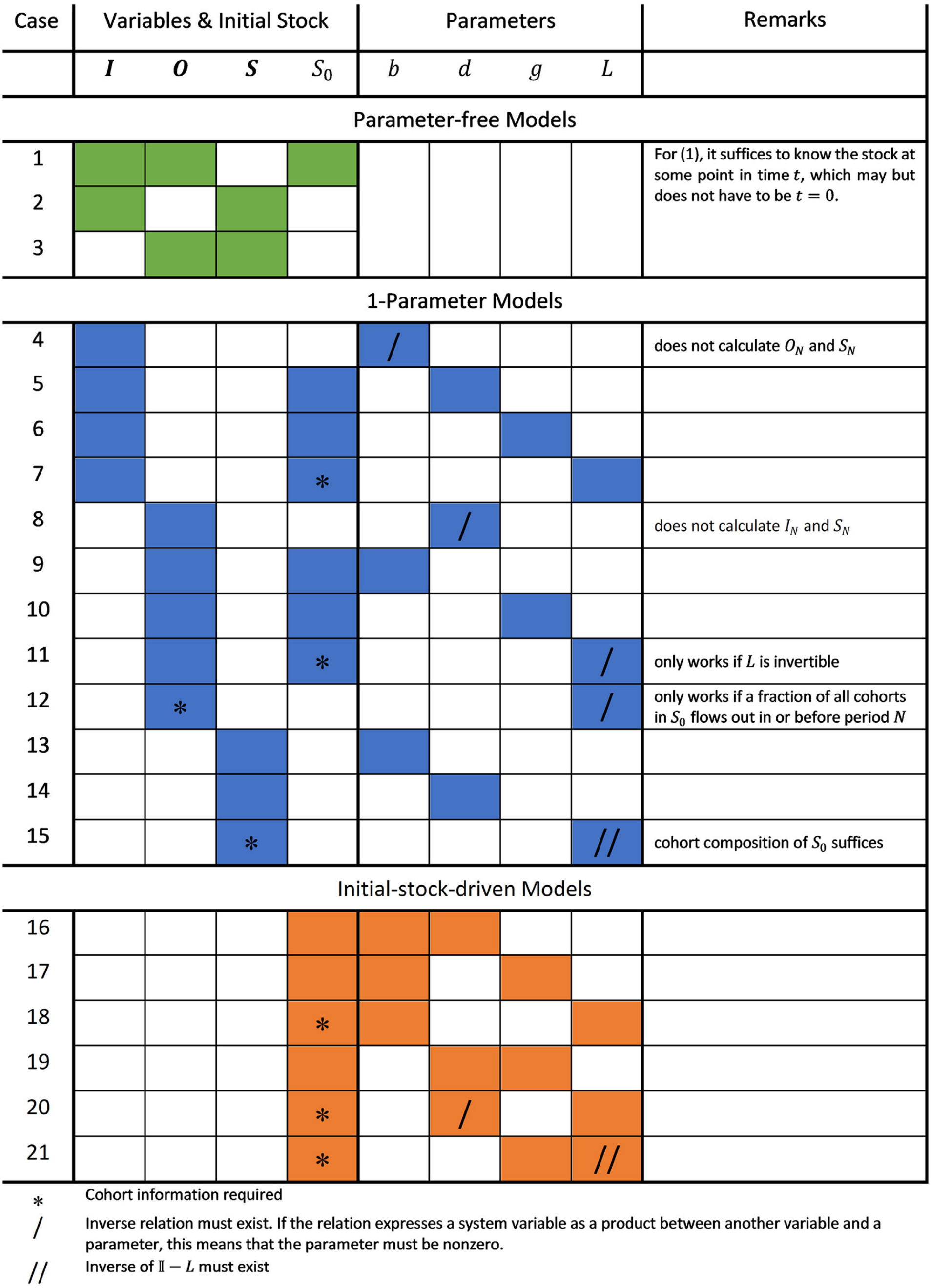

FIGURE 4 The system variables can be determined by combining flow and stock measurements with no model-approach equation (green), one model-approach equation (blue), or two model-approach equations (orange). We distinguish models that rely on the full vector of stock measurements, $\boldsymbol{S}$, including the initial stock, S_0, from models that rely only on S_0

Note that all models using a lifetime and the initial stock as input also require the cohort composition of the initial stock. In general, knowing the cohort composition allows for a more robust estimation of the system variables. In case 11, for example, the inflow can be calculated directly as $\boldsymbol{I} = \boldsymbol{O}L^{-1}$ if the lifetime matrix is invertible. If this is not the case but the cohort composition of the outflow is known, as in case 12, then the inflow of a given cohort c can still be calculated as $I_{c,c} = O_{c,t}/L_{c,t}$ by using an outflow of cohort c during some period $t \geq c$. If however the first outflow of any cohort appears only after having spent τ periods in the stock, then it is impossible to estimate the inflows during the τ last periods of the planning horizon based on outflow and lifetime information alone. This means that the initial stock can only be calculated correctly if a fraction of all its cohorts flows out in or before the last period.

4 | DISCUSSION AND CONCLUSION

The green cases in Figure 4 require little modeling since the balance and intrinsic equations suffice to determine all system variables. However, they require data or assumptions about the initial stock and at least two system variables. If data or reasonable assumptions are available for only one (blue cases) or no (orange cases) system variable, then the remaining variables may be calculated with the help of model-approach equations that link the unknown variables to the known variable or the initial stock. Compared to balance and intrinsic equations, the model-approach equations require less direct information about system variables, but more information about the relationships between them.

4.1 | Choice of model-approach equations

The choice of model-approach equations depends on prior understanding of the system's behavior, on the purpose of the model, and on available data. Thus, a set of model-approach equations cannot be judged in terms of absolute truth, but only by how useful it is in answering predefined research questions. As modelers, we need to assume a causal link between drivers and system variables that is not necessarily present in the real system; this is often a simplification of reality and may create systematic errors.

We name the cases in Figure 4 after the system variables and the parameters they depend on. Since the initial stock is used in almost all cases, we only include it in the name if the case does not depend on any other system variable (as in the orange cases). For example, an estimate of dwelling construction based on housing needs, dwelling lifetime, and the existing housing stock is stock-lifetime-driven. In the following, we compare the use of models in different literature streams based on their driving variables and parameters.

To date, the dynamics of the built environment are mostly described by inflow-lifetime- or stock-lifetime-driven models (Müller, 2006; Pauliuk & Müller, 2014; Müller et al., 2014). The former are particularly useful to model and reproduce the evolution of systems in the past, since data on historic inflows tend to be more easily accessible than data on historic stocks (Chen & Shi, 2012; Chen & Graedel, 2012b; Liu & Müller, 2013). In addition, inflow-driven models tend to be more accurate in the short term because they allow for the modeling of sudden changes such as migration waves or the market penetration of new technologies (Ciacci et al., 2019; Liu et al., 2021). Conversely, stock-driven models, particularly for entities with long lifetimes such as cars or buildings, are well suited for longer-term prospective studies because stocks average out inflow fluctuations and are thus less sensitive to business cycles (Hatayama et al., 2012). In fact, their averaging effect is similar to the one of a low-pass filter in signal processing. In addition, in-use stocks can be seen as a proxy for the level of service, such as housing or transportation, they provide to a population (Müller, 2006; Pauliuk & Müller, 2014; Lin et al., 2017).

Outflow-lifetime-driven approaches are rather uncommon in the MFA literature but very common in perishable inventory management (Fries, 1975; Nahmias, 1977), where the ordering quantities (inflows) depend on demand (outflows) and the residence time (lifetime) of products in the inventory. In addition, outflow-lifetime-driven approaches can be of interest to estimate past inflows and stock sizes based on current outflows and known lifetimes.

Initial-stock-driven approaches are commonly used in system (Forrester, 1968) and population dynamics (Bacaër, 2011). The central premise in these models is that the system is completely described by its initial condition and the laws governing its dynamics, that is, model-approach equations. For example, one might wonder how the size of an animal population evolves given its initial size as well as birth and death rates. Alternatively, one could estimate the depletion of a non-renewable stock such as an ore deposit based on its initial size and extraction rate.

4.2 | Lifetime versus death rate approach

Outflows can be determined using different types of parameter functions in model-approach equations (Figures 2 and 4). The functions either link inflows with outflows through lifetimes, or they connect stock sizes to outflows through death rates. The lifetime approach can be useful if there is evidence that the time span between inflows and outflows follows a robust statistical pattern (Melo, 1999). Estimating such a pattern usually

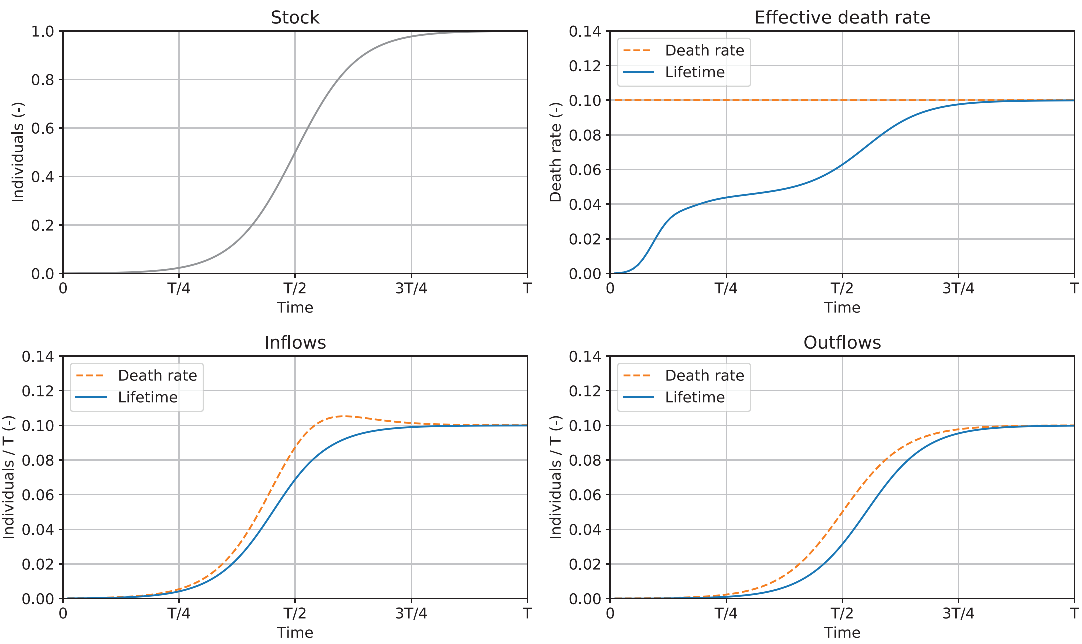

FIGURE 5 Comparison of lifetime- and death-rate-driven models with logistic stock growth and time horizon *T*. The underlying data can be found in the data repository by Lauinger et al. (2021)

requires long-term observations, especially for long-lived entities (Müller et al., 2007; Oguchi et al., 2010; Bongaarts & Feeney, 2013; Kontis et al., 2017). If such a pattern cannot be estimated, an age-independent, possibly time-dependent death rate may still be calculated. Age-independent mortality may be correlated with predation, disease, or adverse environmental conditions for living organisms, and with accidents, natural disasters, or weathering for material goods.

Figure 5 compares the evolution of in- and outflows with a time-invariant lifetime, following a truncated normal distribution, and a constant death rate, equal to the inverse of the mean lifetime, for a model with logistic stock growth. During the initial growth phase, the death rate approach leads to larger in- and outflows than the lifetime approach. The effective death rate of the lifetime approach is therefore lower than the constant death rate. The two rates converge once the stock and its age composition stabilize.

4.3 | Time-varying versus constant lifetime

In general, every cohort may have a different lifetime. In England and Wales, for example, there have been two main changes to human longevity since 1850: (i) infant mortality has decreased drastically, and (ii) adult life expectancy has increased by over 20 years. If historic data about live births are coupled with cohort survival curves, it becomes possible to calculate the deaths of each cohort in each year. This in turn allows us to calculate how many individuals of each cohort are still alive in each year. Figure 6 shows the influence of using an average rather than the actual lifetime for each cohort: the average lifetime overestimates the lifetime of early cohorts and underestimates the lifetime of late cohorts. Initially, the average lifetime approach thus *underestimates* mortality and *overestimates* the size of the population born since 1850. From 1920 onward, the average lifetime approach *overestimates* mortality. From 1950 onward, it *underestimates* the size of the population born since 1850. This leads to wrong conclusions. The average lifetime approach suggests that the population born after 1850 peaked around 1930 and has been declining ever since, whereas the cohort-explicit lifetime approach shows that, in fact, the population has not reached its peak yet and may continue its increase beyond the year 2000.

Conversely, every cohort may have a similar lifetime in a stable environment. For example, human life expectancy between 1770 and 1870 was about 30 years with only slight fluctuations (Zijdeman & da Silva, 2015). In this case it suffices to use an average lifetime for all cohorts.

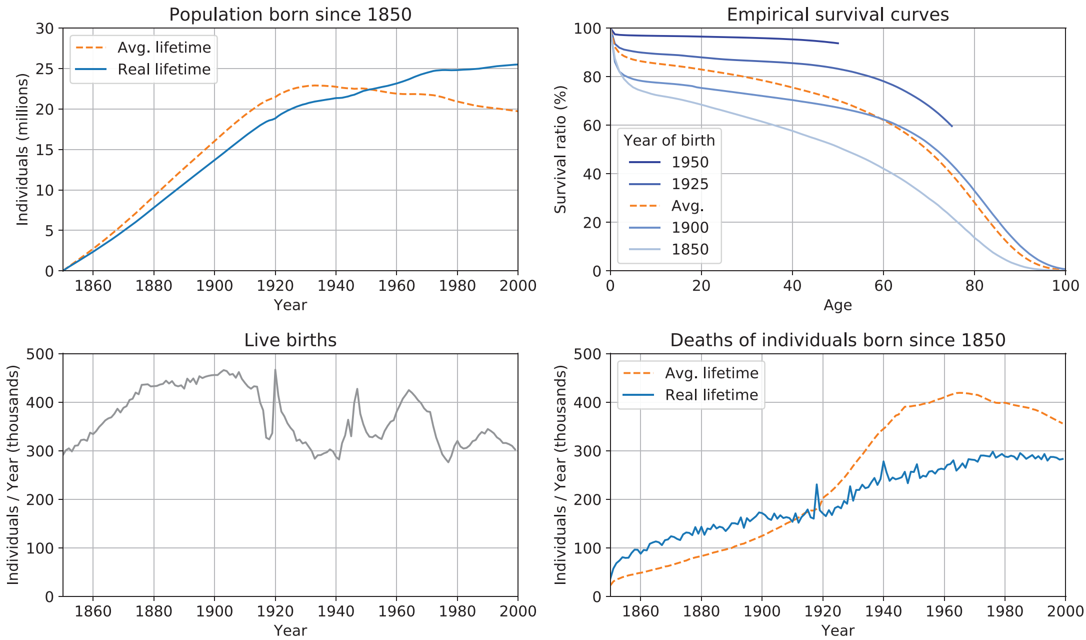

FIGURE 6 Native female population, survival curves, live births, and deaths from 1850 to 2000 for England and Wales. The underlying data can be found in the data repository by Lauinger et al. (2021) and is based on "past and projected data from the period and cohort life tables, 2016-based: England and Wales, 1841 to 2066" by the UK Office for National Statistics

4.4 | Cohorts versus age classes

The effect of time-varying lifetimes can be modeled by distinguishing either cohorts or age classes. While cohort approaches are useful when the properties of individual cohorts are preserved over time (e.g., the material composition of vehicles of a specific cohort is preserved throughout the lifetime of the vehicles, while technological change results in changes in material composition over different cohorts), age-class approaches may be preferable if the properties of a specific age class are robust (e.g., the likelihood of mechanical failure tends to be higher for older vehicles than for newer ones, independent of the cohort). A major difference between the two approaches is that models based on age classes do not always conserve the properties of individuals. For instance, a forestry model distinguishing land parcels by grouping trees into age classes would not conserve the same spatial boundaries over time, as one parcel will keep advancing from one age class to the next. On the other hand, a cohort-based model always keeps track of the same cohort, whose spatial boundaries will remain constant over time. Therefore, properties of individuals and effects of external factors (such as local environmental conditions that may affect growth) are easier to track with a cohort-based model. However, if the age classification reaches the same resolution as the cohorts (at any time t the age of a cohort c is simply t minus c), both approaches can potentially be integrated and thereby preserve balance consistency as well as properties related to both cohorts and age classes.

4.5 | Interdisciplinary learning

We have developed a general framework for stock dynamics and discussed its applications to human populations and to stocks in built and natural environments. The framework can be applied to stocks of any category and has thus the capacity to bridge disciplinary boundaries and to facilitate interdisciplinary learning. It thereby enables comprehensive studies that integrate stocks of human populations and of built and natural environments. The understanding of integrated systems is essential to identify development pathways ensuring human well-being, as it relies upon the "*opportunities that are provided to meet human needs in the forms of built, human, social and natural capital*" (Costanza et al., 2007).

DATA AVAILABILITY STATEMENT

The code and data behind Figures 5 and 6 are available at www.github.com/lauinger/a-general-theory-for-stock-dynamics and on Zenodo (Lauinger et al., 2021).

CONFLICT OF INTEREST

The authors declare no conflict of interest.

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Paper 4

A PRODUCT-COMPONENT FRAMEWORK FOR MODELLING STOCK DYNAMICS AND ITS APPLICATION FOR ELECTRIC VEHICLES AND LITHIUM-ION BATTERIES

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METHODS, TOOLS, DATA, AND SOFTWARE

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A product–component framework for modeling stock dynamics and its application for electric vehicles and lithium-ion batteries

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Abstract

Models that study the socio-economic metabolism often apply a lifetime approach to capture the stock dynamics of products. The lifetime is usually obtained empirically from statistical information and is assumed to describe the dynamics of the product and its components. However, for new types of products for which historic outflow data is limited, or in cases where a critical component plays a significant role in determining product end-of-life, a more refined understanding of the dynamics of product–component systems is needed. Here, we provide a new framework for product–component systems and 12 different approaches to model their stock dynamics. Then, we discuss which approaches are best suited in different contexts. We illustrate the use of the framework with a case study on electric vehicles and their batteries, highlighting the potential of battery replacement and reuse for reducing material demand. Improving the understanding of these complex systems is relevant for the study of the socio-economic metabolism because (i) accounting for component dynamics can support identifying unintended consequences of product-specific policies; (ii) component replacement and reuse can be a key circular economy strategy to foster efficient resource use; and (iii) accounting for these complex dynamics can lead to more accurate estimates for resource demand and waste-generation expectations, creating more resilient information streams. This article met the requirements for a Gold-Gold *JIE* data openness badge described at https://jie.click/badges.

KEYWORDS
circular economy, dynamic modeling, electric vehicles, industrial ecology, material flow analysis, toolbox

1 | INTRODUCTION

Material flow analysis (MFA) has become a prominent modeling tool for understanding how material flows and stocks evolve in metabolic processes in the built environment (Hendriks et al., 2000; Müller et al., 2004). The insights generated using this approach provide an important basis for policy and industry stakeholders in anticipating future anthropogenic activities (Baccini & Brunner, 1991). More specifically, dynamic MFA models seek to build knowledge and foresight about the way different stocks and flows of goods, materials, and energy are used in the socio-economic metabolism and how this changes over time. MFA practitioners often apply a lifetime approach to capture the main driving forces of the stock dynamics as introduced by Baccini and Bader (1996). In-use stocks are composed of products that usually consist of several components, which are assumed to have the same dynamics as the product. This is often not the case in reality; for example, when a component is removed from the product for replacement. Furthermore, this approach can also be limited in cases where critical components in products are an important factor for obsolescence since it does not allow investigating the potential for reuse and replacements to evaluate lifetime extension strategies in sufficient detail.

Several approaches have been put forward in order to deal with such product–component systems. Müller et al. (2004) used different lifetime functions for wood products in buildings and for the buildings themselves to calculate the total wood demand. A similar approach was proposed by Ardente and Mathieux (2014), where two lifetimes are used to test the effect of the durability of two different products, and by Busch et al. (2014), who built an enhanced hierarchical nested description of technologies and their components in which multiple lifetime functions were used to track component outflows in addition to the product dynamics. Furthermore, Sandberg et al. (2014) proposed to consider renovation profiles in buildings to account for changes in the energy intensity of the existing stock, by introducing renovation cycles coupled with the survival curve of the stock-type-cohort matrix. Džubur & Laner (2018) addresses the role of renovation, which can be understood as a critical component of buildings, by adding the demolition and renovation rates in a leaching compared to a lifetime approach. This was further developed by Roca-Puigròs et al. (2020), who proposed a combined lifetime and leaching approach to model the effect of early demolition and renovation strategies for old buildings. To model the dynamics of multiple products containing a common material of interest, Dunant et al. (2021) proposed the use of a transfer function that combines the lifetime functions of different products. However, while these approaches allow to independently track the dynamics of multiple products and components, the combined dynamics and the role of the component in limiting or extending the product's useful time are not considered. Furthermore, the lifetime is usually modeled using the survival function, linking outflows and inflows by tracking the remaining fraction of a given cohort over time (Lauinger et al., 2021). Nevertheless, the life expectancy at birth of an individual does not directly determine the probability of dying in a given year. Similarly, survival functions are not directly linking stocks and outflows.

To address these limitations, we propose a general framework to model the stock dynamics of product–component systems under different conditions. We assume that the lifetime of the product–component system is determined by end-of-life (EOL) of either the product or the component, together with the conditions for product and component reuse and replacement. We introduce a stock matrix by time, product cohort, and component cohort to address these dynamics. We also propose the use of a hazard function to simplify the modeling and establish a direct link between the stocks and the outflows. The interactions of the product–component system can thus be investigated in a detailed way, which allows the evaluation of key circular economy strategies such as reuse and replacement of components.

We present 12 different modeling options, discuss their logics and general relevance for modeling various situations, and provide a specific example with a case study investigating reuse and replacement strategies for batteries in electric vehicles. The Python code for the generic framework is provided and made available for practitioners to use with an open license, building on the foundation laid by Pauliuk et al. (2019) in their work with the dynamic_stock_model library.

2 | FRAMEWORK

This section introduces the different options to model the dynamics of product–component systems. The main differences, applications, and assumptions are discussed from a theoretical point of view. We define products as goods providing a required service, and the components as items within products that are critical to their functionality. The models described in this section are introduced in the Python package product_component_model.py and can be found with its respective documentation here: https://doi.org/10.5281/zenodo.6363382

Following the assumption that the products are providing the required service, and that it is the provision of the service that is driving the demand for the product (Müller, 2006), we use a stock-driven model that allows us to investigate the system dynamics under different modeling assumptions (Lauinger et al., 2021). Figure 1 shows a generic system definition of products and components that allows investigating the dynamics of product reuse and repair by replacing failed components. The spare parts can be assumed to be a new component or a reused component from a failed product. The approach that can be used for a given system may differ depending on the purpose of model and will be discussed in the next section. The proposed methodology is valid for inflow-driven models as well.

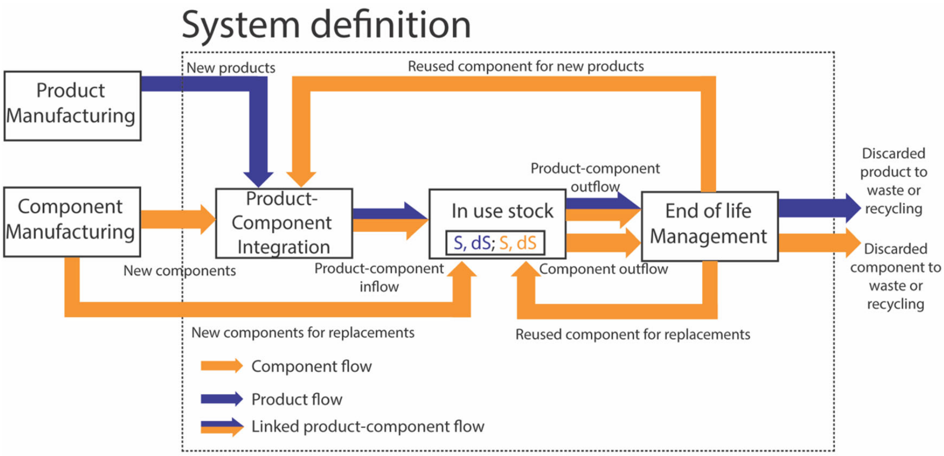

FIGURE 1 System definition of a generic product–component system

2.1 | Considerations about the in-use time and use of hazard functions

Which metric should be used to determine the lifetime of goods? In dynamic MFA studies, the lifetime reflects the statistical probability that a product that entered use at a given time exits use with a specific delay. Therefore, the lifetime does not describe the cause for leaving use, but represents the time interval between when a product enters a balance volume (e.g., use) and when it leaves it to reach EOL. The values used for the lifetime are usually empirically measured, based on sales and waste-generation statistics, or directly measured, and might therefore include periods, when the product is no longer in use but has not reached an EOL reporter yet, known as hibernating stocks. The dynamics of the product and component are assumed to be equal. Therefore, the dynamics of products or technologies where (i) outflow observations are not yet available, (ii) the lifetime of the product and the component is not determined by the same metric, or (iii) where the component dynamics are of relevance to the system should not be characterized in the same way. By considering technical aspects for products, such as kilometers driven by a car, and components, such as number of cycles in a battery, in addition to considerations about other possible causes for obsolescence, we can approximate the useful time of products and components by making use of independent functions.

Component obsolescence can be modeled through a component hazard function, while all other causes for product EOL (including nontechnical failures, such as lifestyle obsolescence) are modeled by a product hazard function. We define the product and component hazard functions as independent functions that describe the theoretical probability of reaching EOL during a given period of time. Despite not having been widely used for dynamic MFA, hazard functions offer significant advantages for the modeling and interpretation of the results and can be derived from statistical lifetime distributions, similarly to the more common survival and probability density functions (see Section 1 in the Supporting Information S1 for a detailed description). Hazard functions determine the time in which the product–component system remains in actual use (providing a service), herein defined as the *in-use time*. Hence, the in-use time varies from the conventional lifetime definition by not including hibernating and obsolete stocks, leading to potentially more accurate inflow but less accurate waste-generation expectations. This relationship holds true in the absence of an additional logic for the hibernating stocks (see Section 2 in the Supporting Information S1). Additionally, given the cohort composition, hazard functions can be used to model the expected outflow of a stock based on its age without requiring previous knowledge of the initial number of inflows, as is the case with the survival function. Thus, the hazard function can establish a direct link between the stock and the outflows (see Section 1 in Supporting Information S1).

2.2 | Modeling options for product–component systems

When evaluating the most suitable approach for a given product–component system, modelers should establish the boundary conditions and limitations around how the component can interact with the product under given circumstances (e.g., whether the component can be replaced or reused). These considerations will not only determine the approach that will be taken, but also the values that should be chosen for the product and component hazard functions.

Figure 2 provides an overview and guide for choosing the most suitable modeling approach to be used dependent on the purpose (and data available). The first consideration is the type of model that is suitable for the problem at hand. This is represented in the uppermost boxes where

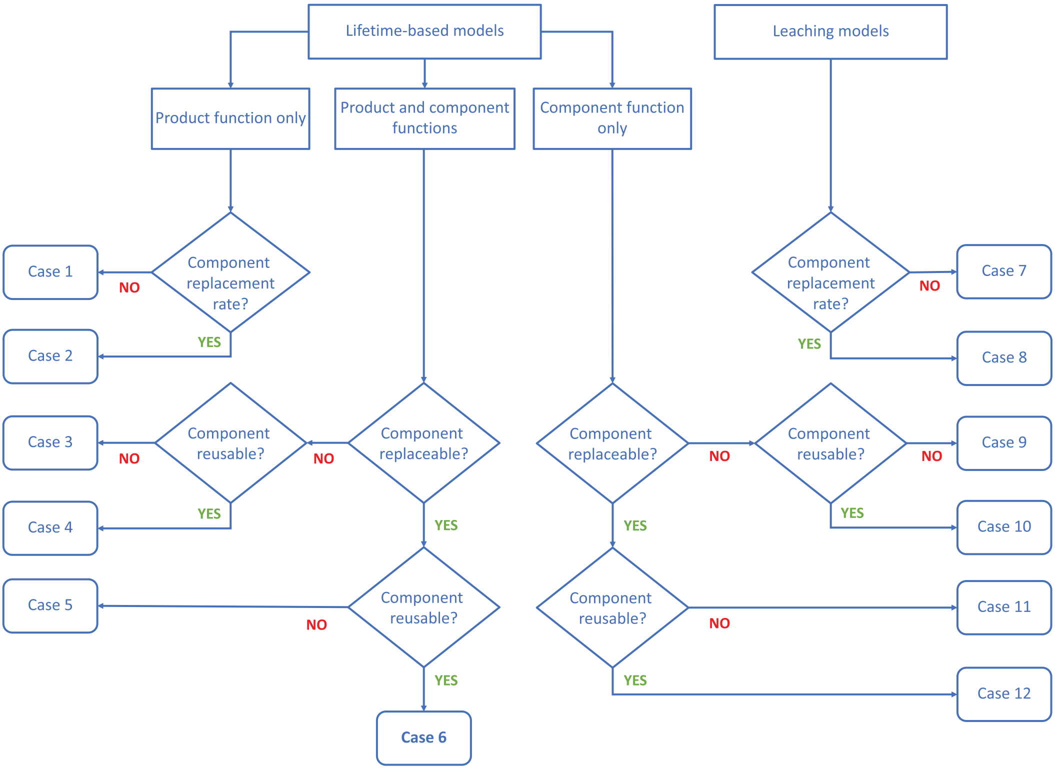

FIGURE 2 Different assumptions for modeling options

lifetime-based models are distinguished from leaching models. Within the lifetime-based models, three main categories are introduced, with several options for reuse and component replacements and will be discussed in detail in the following sections.

2.2.1 | Using a product hazard function

If there is evidence that the relationship between the in- and outflows of goods follows a robust statistical pattern and the dynamics of product–component interactions are not considered or assumed to be equal, a single lifetime approach may be suitable (Melo, 1999). This case can be understood to be equivalent to using only a product hazard function under this framework. The probability distribution of the hazard function is usually calibrated against historical data of inflows or through observations of the size of cohorts over time (survival curve). Examples can be found in products where spare parts are widely available, and components are easy to replace such as lead-acid batteries in vehicles or batteries in consumer electronics.

Case 1: This case depicts the most common approach to dynamic modeling, wherein a single empirical function is used to simulate all outflows. The outflows in this case are calculated based on a probability distribution function of goods flowing out of use given their age. The product and the component are considered inseparable and therefore their system flows are equal. In this case, the product hazard function is equivalent to the lifetime that is traditionally used in dynamic models.

Case 2: In contrast to case 1, here it is assumed that each product uses more than one component through replacements, but it is unknown or irrelevant when the component replacement will be needed. It is therefore assumed that the replacement component enters use at the same time as the product and the first component, and that both components leave use together with the product, leading to a total inflow of components that is always higher than product inflows by an amount equal to the replacement rate. This assumption holds true for constant stocks but leads to an overestimation of the in- and outflows in growing stocks (see Sections 3 and 4 in Supporting Information S1).

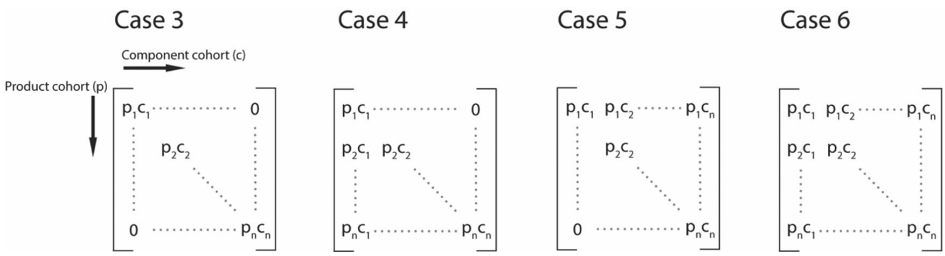

FIGURE 3 Cohort composition of the product–component system for a given time $t = n$ for the different modeling approaches

2.2.2 | Using independent product and component hazard functions

Components may in some cases be a main cause for product obsolescence or contain relevant raw materials, which makes having a refined understanding of their dynamics a pertinent issue. Cases 3, 4, 5, and 6 provide suitable frameworks for this, where the choice of the component hazard function relates closely to the technical aspects limiting its durability, while the product hazard function must also include externalities such as lifestyle choices and accidents relating to the product. This approach allows identifying the outflow of products relating to component and product independently, making it possible to identify strategies for product in-use time extensions and enabling frameworks to avoid planned obsolescence. The strategies for in-use time extension can be tested using the different models under various conditions for component reuse and replacement, which is relevant since for most products there is a market for spare parts, such as tires for vehicles or furniture for buildings. Furthermore, the right to repair is an increasing trend and is an important part of the recently released EU green deal (European Commission, 2019).

Case 3: Here, we introduce the use of component and product hazard functions to estimate the flows of both products and components, as they are considered non-replaceable or reusable. It is assumed that the failure of the component will lead to the obsolescence of the product and vice versa. The in-use time in this case is a composite function resulting from the product and the component hazard functions. The detailed mathematical approach for modeling dual hazard functions and avoiding double-counting issues is described in the documentation of the algorithm. The in-use time of the product and the component, and hence their respective in- and outflows, are equal.

Case 4: Some components might in fact have longer lifetimes than their products and can be reused to build new products once the original one has become obsolete. The separation of product and component flows through the use of independent hazard functions allows the modeler to identify the share of outflows attributed to discarded products that still contain potentially useful components. In a first approximation, we introduce the assumption that a given share of those components is still suitable for further use and can be re-introduced into another new product.

Case 5: This case allows investigating the dynamics of replacing an obsolete component with a new one. Only products that have failed components are considered for a replacement, that is, the outflows related to the component hazard function, so as to not replace the component in an obsolete product. The share of functioning products with failed components that receives a replacement is determined using a component replacement rate.

Case 6: Independent product and component hazard functions are used. Component reuse in addition to component replacements in products already in use is included in this approach. To achieve this, we combine the logics used in cases 4 and 5 to model on the one hand the number of components that can be reused and the number of products that need component replacements. In the case where reused components are not enough to satisfy the demand for replacements, new components are used instead. If too many components are available, then the newest ones will be prioritized, since they are assumed to be in a better state of health.

Figure 3 illustrates the cohort composition of a product–component system for a given time t, where $t = n$ for t in $[t_0, n]$. It can be seen that in case 3, the product and component cohorts are identical, while in case 4 new products may contain older components due to the introduction of replacements with used components. Case 5 shows that older products may contain new components due to replacements, and case 6 combines all these options into a square matrix where a product may contain newer components and where older components may be contained in new products.

2.2.3 | Using inflow/outflow (birth/death) rates

Some goods that exhibit no statistical relationship between their age and the time of outflow or where a share of the total amount is discarded/added every time step independently of age may be better described using rates as drivers. It can be done by introducing product inflow or outflow rates (case 7) and component replacements can be included by using case 8. An important additional shortcoming when using rates instead of lifetimes is the lack of consideration of the cohort composition of the stock and the outflows, as they are calculated as a given share of the total stock. Rates might therefore be better suited for goods that do not have a changing composition over time or for species population investigations where the cohorts are irrelevant.

Since the inflow/outflow rates are linked to the component, in the absence of an additional correction factor, this would assume that no outflows relate to potential product failures, such as accidents. Therefore, the addition of a death rate for the product is considered to address this point.

Case 7: The lifetime approach is fully substituted by calculating the inflows and outflows with birth or death rates, the latter often being referred to as leaching approach (Lauinger et al., 2021). We introduce two cases denominated 7a where a death rate is used as a driver and 7b where a birth rate is used.

Case 8: As an extension to case 7, here we consider no lifetimes and base the flows on either birth or death rates and allow for the component to be replaced at a given rate, which is defined in analogy to case 2.

2.2.4 | Using a component hazard function

In some cases, the dynamics of the components can be considered to be the main limiting factor for the product, e.g. electronical equipment in satellites. Such cases can be approached using cases 9 to 12.

Case 9: Some products might become obsolete if their component fails. Assuming then that the in-use time of the product is mostly determined by the component function, in case 9 the component function is the main driver for the product-component system.

Case 10: Adding complexity to case 9, case 10 depicts a similar situation with the component function being the main cause for outflows but allows for component reuse. Since the component outflows generated by the component's function are by definition obsolete, we assume that none of these components can be reused. However, since the death rate is related to product failures, we define a component reuse rate which determines the share of components that can be reused from failed products.

Case 11: This case illustrates the dynamics of a product whose' component can endlessly be replaced by a new one until the product itself becomes obsolete by a death rate. This could be useful for applications where the component is not critical for the product's in-use time and the product is not the main subject of study, since the cohorts of the same cannot be tracked. Potential examples could be e.g. windows in buildings where the windows are modeled with a given component function and the buildings' dynamics are dictated by a demolition rate. The building would get new windows every time they become obsolete until the building is ultimately demolished.

Case 12: Finally, case 12 can be used as a combined lifetime and leaching approach as described above in analogy to case 11 with further conditions that component reuse and replacements are accounted for using rates.

2.3 | Applicability of the framework

The proposed framework provides greater flexibility in modeling product–component interactions and provides an overview of the modeling considerations that should be taken for product–component systems. The use of independent product and component functions to model their combined dynamics allows a detailed investigation of the consequences of component reuse and replacement strategies. Furthermore, by isolating the cases where obsolescence of the product is caused by the component, different types of data, such as technical specifications, can be used to approximate the hazard functions of new product–component systems where empirical data are unavailable. This might lead to an inflated focus on technical facts, at the expense of more abstract issues, such as consumer behavior and the economics of EOL (Binder, 2007). Therefore, model results should be carefully interpreted and factors external to the measurable causes of obsolescence should be given thorough consideration. The product–component interactions for one component can be addressed using the proposed framework. When several different components are considered, more complex cases can arise, which would require more complex models.

The product_component_model.py library is available to modelers to compute the dynamics of a system for all 12 cases and documentation is provided to facilitate the use.

3 | CASE STUDY: ELECTRIC VEHICLES AND LITHIUM-ION BATTERIES

3.1 | Introduction

The transition toward electric mobility has been a topic of intensive research in recent years due to the quickly growing electric vehicle (EV) production and ever more ambitious national and international targets for electrification (Craglia & Cullen, 2020; IEA, 2021; Xu et al., 2021). This

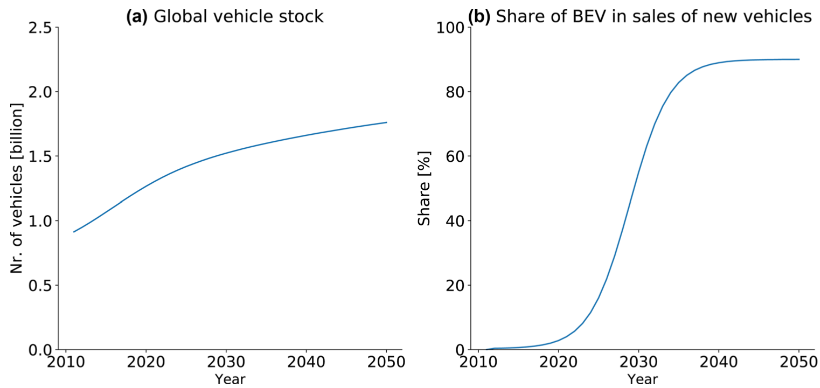

FIGURE 4 Main drivers of the model. Left: The global vehicle stock according to the baseline logistic growth scenario. Right: BEV penetration in the sales according to IEA Net Zero scenario. Underlying data for this figure can be found in Supporting Information S2, file tab "data_for_figure_4_in_manuscript"

shift toward electrification using predominantly lithium-ion batteries (LIBs) results in fundamental changes in the energy demand, resource use, and infrastructure needs globally. From technology metals and rare earths in the LIBs to aluminum for light weighing in the EVs, it is crucial to understand the material needs for both EVs and LIBs as well as options for reuse and recycling (Olivetti et al., 2017).

Given that there are valuable raw materials in both EVs and LIBs and considering that the limitations within the batteries might affect the longevity of the vehicles, EV–LIB dynamics presents a relevant case of product–component interactions where understanding the coupled dynamics is of policy, environmental, and industrial relevance. Moreover, the lack of empirical data on the obsolescence of those goods outlines the need for novel approaches to investigate the dynamics of this system.

We apply the product–component framework presented above to explore the effects of different EOL conditions and strategies on resource use.

3.2 | Methodology

The total stock is calibrated using historical data of registered passenger vehicles from OICA and UN population statistics (International Organization for Motor Vehicles Manufacturers, 201533AD; United Nations Department of Economic and Social Affairs, 2019). From these values, the historical vehicle ownership per capita is derived, which is used to create baseline projections following current trends. The vehicle ownership per capita is multiplied with the baseline UN population projections for 2010–2050 to obtain the total vehicle fleet for that period (see Section 5 in Supporting Information S1).

The global EV fleet (Figure 4a) is calculated using a logistic regression for the share of BEV in sales of new vehicles (Figure 4b) based on the International Energy Agency Net Zero by 2050 report (IEA, 2021). Using cases 3, 5, and 6 as presented above, we calculate the related inflows and outflows under different EOL conditions by defining several scenarios.

Scenario 1 describes a baseline under the current conditions where battery reuse and replacements are not common practice using the modeling approach described in case 3. LIBs are covered by a warranty of 8–10 years (IEA, 2020; Hossain et al., 2019; Tsiropoulos et al., 2018; Vikström et al., 2013); we assume that this is a conservative estimation for the lifetime because manufacturers try reducing liability. We therefore define the component hazard function using a normally distributed curve with a mean of 12 years and a standard deviation of 4 years. Given that EVs have significantly fewer moving parts than conventional vehicles and lack the main part causing ICE EOL—the engine—we assume a comparatively longer lifetime of 18 years with a standard deviation of 4 years (Jung et al., 2018; Oguchi & Fuse, 2015; IEA, 2019). This value is intended to reflect technical aspects as well as accidents and lifestyle choices of the vehicle owners.

Scenario 2 is defined to investigate the role of battery replacements strategies. We use the modeling approach described in case 5. This allows us to model the EV and LIBs flows if a share of faulty batteries can be replaced by new batteries, thus avoiding the early obsolescence of the vehicle. Furthermore, with this approach we show the change in EV and LIB demand depending on how widespread the practice of battery replacement becomes. To illustrate this, we compare the results of introducing a 30% replacement rate to an 80% replacement rate.

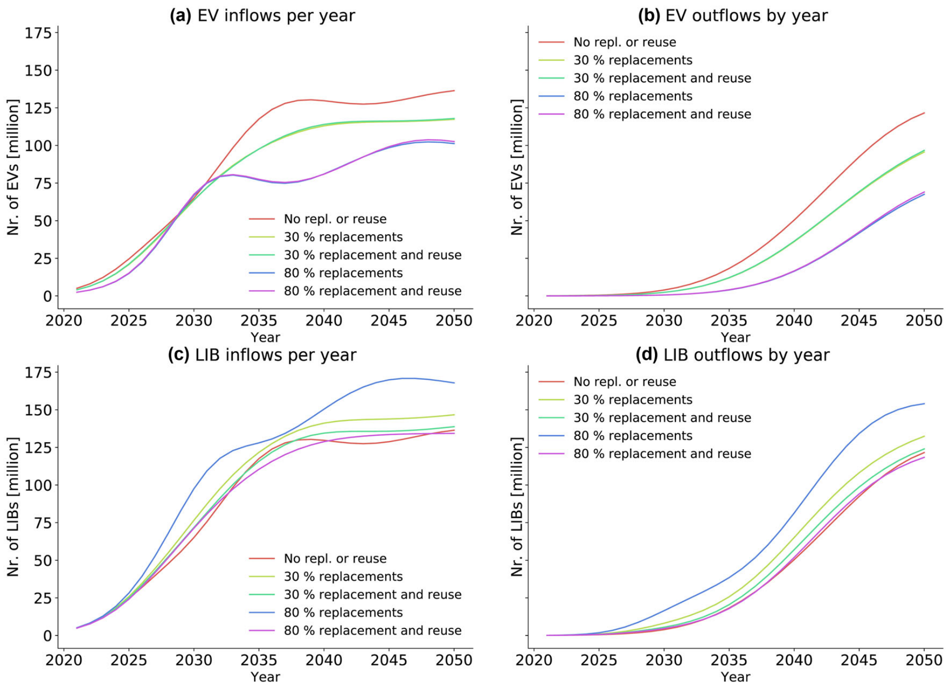

FIGURE 5 (a) EV inflows for the various scenarios, (b) EV outflows for the various scenarios, (c) LIB inflows for the different scenarios, (d) LIB outflows for the different scenarios. Underlying data for this figure can be found in Supporting Information S2, file tab "data_for_figure_5_in_manuscript"

Scenario 3 addresses another intervention that could re-shape the use of LIBs: The reuse of batteries from vehicles that were decommissioned due to car failures such as crashes, but that are still in a good state of health. These batteries could be used for battery replacements in vehicles that are already in the fleet, provided they are in good state of health. We use the methods described in case 6 to calculate the mass flows with a 30% reuse and replacement rate and an 80% reuse and replacement rate.

3.3 | Results

Figures 5a and 5c show the demand for EVs and LIBs for the different modeling assumptions, respectively. It can be seen that the highest EV demand corresponds to scenario 1 in which no replacements or reuse are considered and is simultaneously the case with one of the lowest LIB demands.

After introducing battery replacements, the demand for EVs and LIBs shows that while the LIB demand is increased compared to findings without replacements, the EV demand is reduced. This highlights the fact that the batteries can severely limit the vehicle lifetime, which in turn has significant consequences for resource use. This effect is stronger, the higher the replacement rates (see yellow and blue curves).

Finally, introducing reuse in combination with replacements shows that while this strategy does not seem to have a significant impact on the demand for EVs as compared to the scenario with only replacements, the demand for LIBs is significantly reduced to levels comparable to the findings without replacements. This highlights the synergistic effects that a combined replacement and reuse strategy has on minimizing the resource use of both EVs and LIBs. If the replacement and reuse practices are increased from 30% to 80%, the LIB demand is not affected in a significant way, but the EV demand is further reduced as can be seen in Figure 5a. The non-sensitivity of the LIB flows to these parameters is caused by the large difference between product and component lifetimes, where one EV can in most cases accommodate the use of two new LIBs throughout its lifetime and therefore the outflowing LIBs are in poor state of health and unsuitable for reuse in the fleet. Figure 5b,d shows the corresponding outflows to each modeling case and the survival curves of the first cohort for each case can be found in Section 5 in Supporting Information S1.

3.4 | Discussion

Using the novel methodologies proposed in this paper, an improved understanding of product–component interactions has been presented. Electric vehicles are new products for which empirical data on obsolescence is limited. However, the use of product and component hazard functions allows estimating the in-use time of EVs and LIBs using technical data under different EOL conditions. This results in more robust estimations on resource use and allows the investigation of key circular economy strategies such as repair and reuse of components.

3.4.1 | The role of battery replacement

Since EVs have significantly fewer moving parts, their technical lifetime could be expected to exceed that of an internal combustion engine vehicle, LIB limitations aside. The results show that implementing widespread battery replacements can trigger an effective in-use time extension for the vehicles, which leads to a significant reduction in vehicle, and thus raw material, demand. However, if this strategy is not combined with a widespread battery reuse strategy, it might result in an increased demand for batteries.

Extending the requirements for the duration of battery warranty may be an incentive for manufacturers to extend battery lifetime or to facilitate replacements and repairs. Additionally, informing customers about expected lifetime and repair options could orient purchasing decisions toward more durable goods, and eventually improve the design standards of the industry.[1] Standardization of parts can help the ease of repair and reduce costs, although it might be challenging to achieve given the high competitiveness and quick development of the industry. Furthermore, the risk of planned obsolescence of vehicles by means of limiting battery lifetime and replacements can be reduced by these practices.

Research suggests that durability is preferred in leasing business models (Pangburn & Stavrulaki, 2014), but only if take-back costs of the battery are sufficiently low (Zhu et al., 2021). Therefore, stringent regulations or customer demand for battery replacements may encourage manufacturers to develop new business models such as leasing, where they retain ownership of the batteries and sell a service instead of a product.

3.4.2 | Cost of battery replacement vs. residual value of the vehicle

At present, new battery costs are prohibitively high for battery replacements to be widely adopted, apart from cases where they are covered by warranty. Therefore, as has been shown in scenario 1, consumers might be incentivized to discard their vehicles once the battery fails, even if the vehicle itself would in theory still be in good. This could be addressed by policymakers through the introduction of subsidies or incentives targeted to the batteries themselves instead of only incentivizing EVs. For instance, in Norway, EVs benefit from VAT exemptions, but LIBs do not (Thorne et al., 2021), often rendering the residual value of the vehicle to be lower than the cost of a new battery. This results in an early outflow of the vehicle and can be relatively easily avoided by encouraging car owners to replace their batteries rather than discarding both vehicles and batteries, as presented in scenarios 2 and 3.

3.4.3 | The role of battery reuse

Scenario 3 showed that a widespread adoption of battery reuse could lead to a beneficial synergy with the battery replacement practice that helps reduce the demand for both EVs and batteries. The demand for batteries when reuse is implemented is lowered significantly compared to when only replacements are introduced, and even more compared to when none of these practices are used, as shown in scenario 1. Some challenges may arise regarding the responsibility in case of failure of second-hand batteries in EVs, due to the limited transparency about the state of health of second-hand batteries and the lack of standardized processes for manufacturers and insurance companies. A reliable assessment of the state of health of the battery, clear responsibility guidelines, and a resilient reverse logistics system need to be designed to enable replacements with used batteries.

4 | CONCLUSION

In the transition to a sustainable society, key circular economy strategies include reuse and lifetime extension of products and components. In order to understand the intended and unintended consequences of such strategies, it is essential to adequately represent the dynamics of product–component interactions in MFA models. This is relevant for both policymakers to better understand the impact of interventions and for industry stakeholders to plan their infrastructure to not only meet the demand but also to deal with EOL goods.

The product–component framework proposed in this manuscript expands on current practices for dynamic modeling by differentiating alternative approaches to mode product–component relationships. It provides an overview of alternative approaches and a guide for the user in selecting the approach best suitable for the specific conditions. The product–component framework is made fully available to researchers in generic code that can be further refined for specific cases. Building on these methods, researchers can contribute to deepen the knowledge base for policymakers and industry stakeholders by investigating key circular economy strategies, such as repair and reuse, using more refined and sound approaches that consider the interlinked dynamics of product–component systems.

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CONFLICT OF INTEREST

The authors declare no conflict of interest.

DATA AVAILABILITY STATEMENT

Data openly available in a public repository that issues datasets with DOIs; see https://github.com/fernaag/product_component_model.

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[1] The UN has recently expressed the importance of this aspect; the statement can be found in the downloads here: https://unece.org/transport/documents/2021/03/working-documents/iwg-eve-proposal-new-un-gtr-vehicle-battery

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SUPPORTING INFORMATION

Additional supporting information can be found online in the Supporting Information section at the end of this article.

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Paper 5

EVALUATING STRATEGIES FOR MANAGING RESOURCE USE IN LITHIUM-ION BATTERIES FOR ELECTRIC VEHICLES USING THE GLOBAL MATILDA MODEL

Fernando Aguilar Lopez, Romain G. Billy, and Daniel B. Müller

Resources, Conservation & Recycling (under review)

This paper is awaiting publication and is not included in NTNU Open

Paper 6

ALUMINIUM USE IN PASSENGER CARS POSES SYSTEMIC CHALLENGES FOR RECYCLING AND GHG EMISSIONS

Romain G. Billy and Daniel B. Müller

Resources, Conservation & Recycling (under review)

This paper is awaiting publication and is not included in NTNU Open

Paper 7

PATHWAYS TOWARD A CARBON-NEUTRAL SWISS RESIDENTIAL BUILDING STOCK

Marta Roca-Puigròs, Romain G. Billy, Andreas Gerber, Patrick Wäger, and Daniel B. Müller

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RESEARCH

Pathways toward a carbon-neutral Swiss residential building stock

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Abstract

Current policies to reduce energy consumption and CO_2 emissions associated with buildings focus on technological developments such as energy efficiency, renovation rates and renewable energies. While technological developments are effective at mitigating climate change, the omission of lifestyle changes such as lower floor area per capita and indoor temperatures as well as disruptive measures (*e.g.* replacement of highly energy-consuming buildings) leave untapped potential for further savings. A dynamic stock-driven model is presented that quantifies direct energy consumption and direct CO_2 emissions associated with the use phase of Swiss residential buildings. Eleven scenarios involving technological developments, lifestyle changes and disruptive measures are evaluated against relevant goals (Paris Agreement, Energy Strategy 2050 and 2000-Watt Society). Disruptive measures are modelled with a new combined lifetime-leaching approach. The scenario analysis indicates that the main leverage points for energy savings reside in lifestyle changes, whereas emission reductions can be highly levered by technological developments. Reaching all the goals is possible, but requires ambitious strategies. This study provides a basis for expanding the portfolio of climate change mitigation strategies for the residential building sector, although further research is needed to understand social, cultural and economic aspects, and indirect (embodied) emissions.

Policy relevance

Switzerland currently applies two policies in the building sector to reach the climate goals (Energy Strategy 2050, Paris Agreement and 2000-Watt Society). This study shows: (1) current policies (a CO_2 levy on fossil fuels for heating and the Buildings Program subsidising renewable energies and energy-efficient renovations) are effective at lowering energy consumption and CO_2 emissions, but insufficient to meet any of the goals; (2) reaching the Energy Strategy 2050 and Paris Agreement requires an extension of current policies and a complete phase-out of fossil fuels by 2050; and (3) achieving the 2000-Watt Society requires the measures described above, households heating only areas inside dwellings up to 20°C, and one of these three measures: (a) households living with 41 instead of 47 m^2/cap, (b) increasing the renovation rate from 1.3% to 3.0%, and (c) replacing buildings consuming > 140 kWh/m^2/yr. Further evaluations including social, cultural and economic aspects, and indirect energy consumption and embodied emissions are needed.

Keywords: building stock; climate change; combined lifetime-leaching approach; dynamic material flow analysis (MFA); mitigation strategies; scenario analysis; Switzerland

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1. Introduction

Many governments have set CO_2 emissions and energy-reduction goals and developed action plans to mitigate the potentially catastrophic consequences of climate change. The building sector plays an important role in these action plans due to its high CO_2 emissions and energy consumption. Although available and affordable low-carbon technologies make the sector attractive, the long lifetimes of buildings require long-term management strategies (Bauermann 2016; Kohler 2017). Worldwide, energy and emissions stemming from the operation of buildings are responsible for 31% of total annual energy consumption and 8% of total annual CO_2 emissions; when emissions associated with electricity production are included, these emissions account for 23% (IPCC 2018).

Strategies to reduce direct energy consumption and CO_2 emissions associated with the use phase of buildings vary widely, but can be categorised as technological developments (energy efficiency, renovation activities, energy mix) and lifestyle changes (indoor temperatures, size of dwellings). The existing literature for various countries and regions shows that future energy and emissions could be substantially reduced by the following technological developments: increasing the frequency of renovation (2–3% yearly renovation rates), increasing the use of photovoltaics and heat pumps, and improving the energy performance of existing and new buildings (Bauermann 2016; Bettgenhauser & Hidalgo 2013; Charlier & Risch 2012; Economidou *et al.* 2011; Firth *et al.* 2010; Meijer *et al.* 2010; Müller 2015; Pauliuk *et al.* 2013; Sandberg *et al.* 2017; Serrenho *et al.* 2019; Vásquez *et al.* 2016). Lifestyle changes are less prominent in the current literature; however, existing research indicates that a smaller floor area per capita (FApC) and lower indoor temperatures could contribute considerably to meeting climate targets (Pauliuk *et al.* 2013; Sandberg *et al.* 2017; Serrenho *et al.* 2019).

Current policies for national building stocks tend to address climate change through technological developments only, which evidences the untapped savings potential of lifestyle changes. Additionally, disruptive measures such as replacing the entire building stock by 2050 have been found to reduce direct energy consumption and emissions substantially (Pauliuk *et al.* 2013; Serrenho *et al.* 2019). However, the concomitant increase in construction activity and indirect environmental impacts make these disruptive measures unreasonable. Nevertheless, an increased replacement of only the most energy-consuming buildings by highly energy-efficient ones could result in long-term energy and emissions savings, given that the environmental impacts of construction would be offset by substantial savings of direct energy and emissions. To the authors' knowledge, disruptive measures triggering the replacement of only a specific segment of the stock have not yet been considered in the literature.

In Switzerland, operating buildings accounts for 27% of total CO_2e emissions and 28% of total energy consumption (FOEN 2019b; SFOE 2019). Switzerland has two central energy-related goals: (1) the Energy Strategy 2050 (ES2050) with per capita energy reduction targets for 2020, 2035 and 2050 of 16%, 43% and 54%, respectively, compared with the year 2000 (SFOE 2018b); and (2) the 2000-Watt Society envisioning 2000 W of primary energy use per person in 2050, in terms of continuous power (Stulz *et al.* 2011). Regarding emissions, the main goals are: (1) the Kyoto Protocol with a 40% reduction by 2020 compared with 1990 (FOEN 2018a); and (2) the Paris Agreement, which aims at carbon neutrality by 2050 (FOEN 2019a). To reach these goals, Switzerland applies the following policies specific to the building sector: (1) a CO_2 levy on heating oil, natural gas and coal; and (2) a Buildings Program (BP) subsidising the transition toward renewable energies and energy-efficient renovations (FOEN 2018b).

The literature on energy and emission reductions for the Swiss residential building stock shows that the energy goals could be reached by a 50% decrease of space heating demand in 2050 compared with 2005, and by heat pumps and solar energy supplying about 70% of the total energy demand in 2050; the reduction in space heating demand could be achieved through high energy-performance standards and high retrofitting rates (2%) (Drouilles *et al.* 2017; Heeren *et al.* 2013; Kost 2006; Pfeiffer *et al.* 2005; SFOE 2016; Siller *et al.* 2007; Wallbaum *et al.* 2009; Wang *et al.* 2018). The scarce literature on lifestyle changes indicates that a 25% reduction in FApC could decrease energy by 10% and emissions by 25% in 2050 compared with 2005 (Drouilles *et al.* 2017). Existing studies often neglect the performance gap between the theoretical or technical energy performance of buildings and real energy consumption by households, which according to the results of Schneider *et al.* (2017) could lead to 20% higher energy demand in 2050. Much of this gap could be reduced if households used energy responsibly (lower indoor temperatures) (Khoury *et al.* 2017).

The limited consideration of lifestyle changes and the lack of scenarios portraying disruptive measures highlight the potential to expand the Swiss portfolio of climate change mitigation strategies for the building sector. An extension of the portfolio could improve decision-making processes under adverse futures. Therefore, the main goal of this contribution is to inform policy-makers in the Swiss residential building sector of alternative strategies (including technological developments, lifestyle changes and disruptive measures) to meet the energy and emissions goals. The following research questions will be addressed:

- How can disruptive measures be modelled, such as increased replacement of the most energy-consuming buildings by highly energy-efficient buildings?
- What are the main leverage points in the Swiss residential building stock to reduce energy and emissions?
- What measures are needed for the Swiss residential building sector to reach the energy and emissions goals?

To answer these questions, the authors developed a dynamic stock-driven model to quantify direct energy consumption and direct CO_2 emissions associated with the operational phase of Swiss residential buildings. Disruptive measures are modelled with a new combined lifetime-leaching approach, and 11 scenarios are evaluated, including technological developments, lifestyle changes and disruptive measures, against the Swiss energy and emissions goals.

2. Methods

2.1 System definition

The system describes the use phase of residential buildings with the following aspects: floor area, direct energy consumption and direct CO_2 emissions (**Figure 1**). Given that these aspects are closely coupled with each other, the system contains one multilayered process representing the use phase of residential buildings with three layers: floor area, energy and emissions. The *floor area layer* quantifies the stock of living area and the stock of energy reference area (ERA). According to the Swiss Society of Engineers and Architects, the living area accounts for the area available for the occupant(s) inside the dwelling, and the ERA accounts for the effective heated area including areas beyond the dwelling area (*e.g.* staircases, attics, basements) (SIA 2007). Furthermore, the floor area layer quantifies the inflow (construction), outflow (demolition) and stock change associated with the stock of living area.

The stock is segmented by cohorts (construction years), building types, renovation states and intensity of use. Historical cohorts are defined following the official classification, and the length of future cohorts is set to 10 years, corresponding to recent historical cohorts (see Appendix A in the supplemental data online). The building types are segmented into single-family houses (SFH) and multi-family houses (MFH). Three renovation states were differentiated reflecting the improvements in energy efficiency: non-renovated (R1), renovated with the technologies available between 1971 and 2020 (R2) (1971 marked the beginning of energy-efficient renovations, and 2020 was considered as the current year), and renovated with the technologies available after 2020 (R3) (scenario specific). The use of the stock was segmented by three intensities: stock used daily (U1), stock used temporarily (U2) and vacant stock (U3).

The *energy layer* quantifies the direct demand for useful and final energy. The energy demand accounts separately for space heating (SH), domestic hot water (DHW) and other uses (lighting, electric appliances, ventilation, air-conditioning

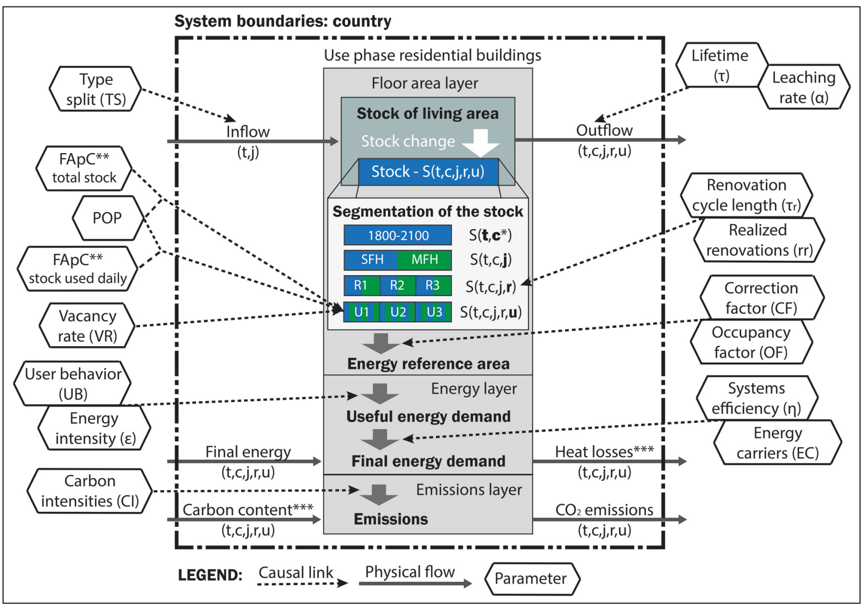

Figure 1: System definition and model description for the use phase of residential buildings, including floor area stock, direct energy consumption and direct emissions. System variables: stock, stock change, inflow, outflow, energy reference area (ERA), useful energy, final energy and CO_2 emissions.

Notes: Dimensions: t = time; c = cohorts; j = building types (SFH = single-family houses; MFH = multi-family houses); r = renovation states (R1 = non-renovated; R2 = renovated during 1971–2020; R3 =renovated after 2020); u = intensity of use (U1 = used daily; U2 = used temporarily; U3 = vacant). Parameters: POP = population; FApC = floor area per capita for total stock and stock used daily; TS = type split; τ_r = renovation cycle length; rr = realised renovations; VR = vacancy rate; CF =correction factor; OF = occupancy factor; UB = user behaviour; ε = energy intensity; η = heating systems efficiency; EC = energy carriers; and CI = carbon intensity.

* Cohort segmentation is not visualised.

** FApC is calculated by two additional parameters: FApD = floor area per dwelling; and PpD = people per dwelling.

*** Heat losses and carbon content are not explicitly calculated in the model; they are shown for the unit consistency of each layer.

and minor uses). Cooking accounts for 3% of the total energy consumption in buildings (SFOE 2018a), and it was not included due to poor data availability. Following SFOE (2018a), the energy carriers considered were heating oil, natural gas, coal, direct electricity, electricity for heat pumps, wood, renewables (solar energy), district heating and others. The *emissions layer* provides the direct CO_2 emissions; therefore, other greenhouse gas emissions are not accounted given that CO_2 accounts for 99% of the CO_2e emissions associated with the use phase of residential buildings (FOEN 2019b).

2.2 Model description

The stocks and flows were calculated using a dynamic stock-driven model in which population and FApC define the stock of living area. The model formulation was based on a series of publications (Müller 2006; Sandberg *et al.* 2016, 2017; Vásquez *et al.* 2016). The entire model formulation is presented in Appendix B in the supplemental data online, and the differences between the model and those described in the existing literature are provided below, and summarised as the segmentation of the stock by intensity of use and the combined lifetime-leaching approach.

Siller *et al.* (2007) found differences between statistical data and model results, which could be explained by the omission of the intensity of use of the stock. The model tackles this by calculating two FApC: (1) that accounting for the total stock; and (2) that accounting for stock used daily. In both cases, FApC was obtained by dividing the floor area per dwelling by the people per dwelling. Each FApC was multiplied by the population to obtain the total stock and the stock used daily (both stocks in terms of living area). The vacant stock was obtained by multiplying the vacancy rate by the total stock. The stock used temporarily was determined by subtracting the vacant stock and the stock used daily from the total stock. The stock of ERA was calculated using the method described by Streicher *et al.* (2019) (**Figure 2A**), which resulted in ERA1 and ERA2 depending on the stock of the living area used (**Figure 2B**). This study additionally calculated the stock of ERA as the sum of the stock used daily and the stock used temporarily corrected by the occupancy factor (ERA3).

The combined lifetime-leaching approach was developed to explore disruptive measures by using the existing lifetime and leaching approaches. Buildings stock models assume that the demolition of the stock is either determined by a predefined building lifetime (lifetime approach) or by a demolition or leaching rate (leaching approach) (Bauermann 2016; Müller 2006; Van der Voet *et al.* 2002). While the lifetime approach considers the heterogeneity of the stock (cohort or age structure), it has limitations with respect to representing disruptions of the predefined building lifetime such as age-independent demolition. The leaching approach calculates demolition as a fraction of the stock; therefore, the stock is considered homogeneous and demolition is independent of the cohort structure, which may lead to inaccurate results. However, the leaching approach allows immediate growth of the demolition activity to be modelled by increasing demolition rates. Both approaches have their strengths, weaknesses and areas of application; therefore, a novel approach is proposed in which the strengths of the two are combined. The natural ageing process of a heterogeneous stock is accounted for by the lifetime principle, while the leaching approach captures the age-independent outflows triggered by the increased replacement (disruptive measure). The age-independent outflows are determined by multiplying a leaching rate, which is targeted at a segment of the stock, by the stock. The targeted segment of the stock was assumed to have no lifetime-related outflows during leaching. For the mathematical formulation of the combined approach, see Appendix C in the supplemental data online.

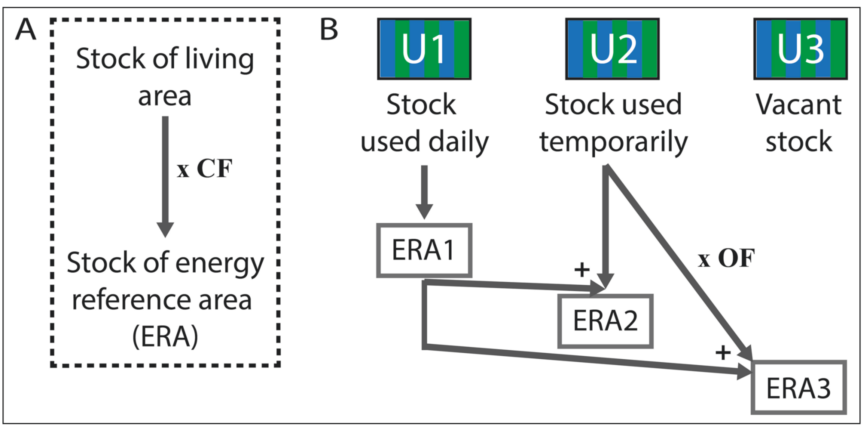

Figure 2: Energy reference area (ERA)-related calculations. **(A)** Generic ERA calculation from the stock of living area using a correction factor (CF) that accounts for heated areas beyond the dwelling area. **(B)** ERA approaches used in this study: ERA1 obtained from the stock used daily; ERA2 obtained from the stock used daily and temporarily considered as stock used daily; and ERA3 obtained from stock used daily and temporarily corrected by the occupancy factor (OF).

The model was implemented using Python by adapting the library Open Dynamic Material Systems Model to include types, energy, emissions and the combined lifetime-leaching approach (Pauliuk & Heeren 2020).

2.3 Parameter estimation and uncertainty analysis

The model description is generic; thus, it could be adapted to different system boundaries. In this study, the Swiss national borders define the spatial system boundaries and a simulation time of 301 years, 1800–2100, is applied. The overview of the input data, parameter assumptions and calibration for the most relevant parameters is provided in **Table 1** (for the complete table and specifications see Appendix D in the supplemental data online). In line with the findings of Naber *et al.* (2017) regarding predominant uncertainty analyses in building stock models, an uncertainty analysis, including two sensitivity analyses (SA) and comparative analyses, was performed. Two SA were conducted to study the effects of a one-factor-at-a-time (OFAT) parameter variation (±10%) in either the historical input data or the future development of the parameters. Similarly, as in Sandberg *et al.* (2016), for the historical parameter variation, the parameters were classified as having either high or low uncertainty depending on the data sources used (**Table 1** and see Appendix D in the supplemental data online), the SA was performed with the parameters evaluated with high uncertainty and the results were evaluated for 2020. The parameter variation for future input data was carried out for all parameters except for the carbon intensities of heating oil, natural gas and coal, given that they are determined by the carbon content of the fuel, which is expected to remain unchanged (for details, see Appendix D in the supplemental data online). The results were analysed for 2050. For the two SA, the results were calculated as relative sensitivities (relative change in output over relative change in input) (for the equation, see Appendix D in the supplemental data online). The comparative analyses were conducted to validate model results against statistical data and similar studies.

2.4 Scenarios

A scenario analysis was conducted to assess the strategies for reducing direct energy and emissions stemming from the operation of Swiss residential buildings. The results were evaluated against the goals presented in section 1. The conceptual outline and description of the scenarios are presented in **Figure 3**; for a detailed description of the goals and scenarios, see Appendix E in the supplemental data online.

The scenarios were built considering a cumulative aspect and two types of scenarios. The cumulative aspect is illustrated in **Figure 3** by arrows indicating how the scenarios build on each other (*e.g.* carbon neutrality considers the premises in extend Buildings Program). The two scenario types are forecasting and backcasting.

The baseline scenario was defined with current policies in place, assuming the end of the BP in 2025 (currently planned). An extension of the programme was explored in the extend Buildings Program scenario. Given that the Swiss government has officially committed to carbon neutrality and the ES2050 goals, a backcasting scenario, carbon neutrality, was built to explore how the two goals can be reached.

The forecasting energy-reduction scenarios explore ambitious measures to reduce energy consumption in buildings further. While the green lifestyles scenario analyses two lifestyle changes (a gradual shift from average indoor

Table 1: Description of the most relevant parameters. The source corresponds to the values and assumptions.

Parameter	Value	Sources	Assumptions	Evaluation of data uncertainty
Population	See Appendix D	FSO (2018b), HSSO (2012b), UN (2019)	Medium projection	Low
Floor area per dwelling[a]	See Appendix D	Bergsdal *et al.* (2007), FSO (2000, 2018c)	65 m^2/dwelling in 1800 104 m^2/dwelling in 2100	Low
People per dwelling[a]	See Appendix D	FSO (2017), HSSO (2012a), Müller (2006)	5 people/dwelling in 1800 2 people/dwelling in 2100	Low
Lifetime	200 years	Kornmann & Queisser (2012)	Lifetime was assumed equal for all cohorts and types, and was found through a process of calibration and validation (see Appendix D)	High
Renovation cycle length	40 years	Filchakova *et al.* (2009)	Renovation cycle length equal to the longest lifetime of energy-relevant building components	High

Notes: [a] Stock used daily.
For appendices, see the supplemental data online.

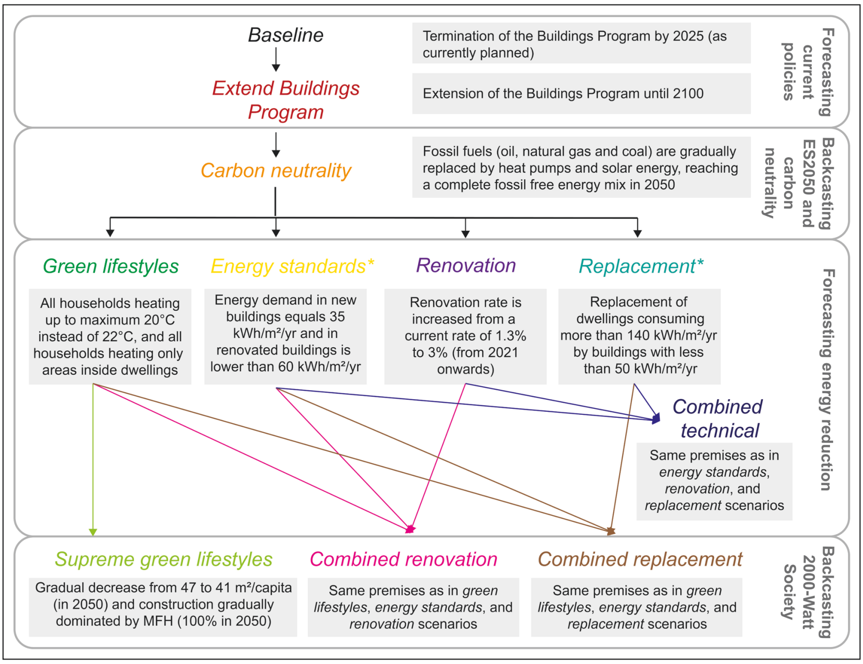

Figure 3: Conceptual outline of the scenarios.

Note: Arrows between scenarios indicate how the scenarios build on each other. The premises are specified in the grey boxes. The scenario typology (forecasting or backcasting) is presented on the right side. * Energy values are given for useful energy.

temperatures of 22 to 20°C and gradual avoidance of heating up areas outside dwellings), the energy standards, renovation and replacement scenarios investigate individual technological measures: best energy standards for new (Minergie-A) and renovated buildings (Minergie-P) (Minergie 2020), increased renovation rate and gradual replacement of dwellings with the highest energy demand by energy-efficient dwellings during the period 2021–30, leading to their complete replacement by 2030. A combination of the three technological measures was analysed in the combined technical scenario. The 2000-Watt Society goal was investigated with three backcasting scenarios: supreme green lifestyles, combined renovation and combined replacement. While highly ambitious lifestyle changes (lower FApC and construction linearly dominated by MFH) were studied in supreme green lifestyles, the combined renovation and combined replacement scenarios explored combinations of technological measures together with less ambitious lifestyle changes. The scenario results beyond 2050 are highly uncertain; therefore, they are presented but not discussed.

3. Results

3.1 Baseline scenario and uncertainty analysis

According to the baseline scenario, the Swiss residential building stock is expected to grow until 2100; however, the growth toward the second half of the 21st century will slow down (**Figure 4**). The expected stock growth is driven by a projected increase in population, given that FApC was assumed to stagnate at current levels. Simulation results for construction show an increase until 1975 with strong growth after the Second World War, a decrease in 1975–2075, and a small increase for the last 25 years simulated. The results for demolition present a flat trend until 2025 and a subsequent increase. The decrease in construction after 1975 and the low demolition activity are driven by the long lifetime of dwellings. The historical results of the stock, inflow and outflow fit the overall trends of the statistical data well; however, they fail to capture the short-term fluctuations of construction and demolition activities.

The results of the stock segmented by renovation states were equivalent to a renovation rate of 1.3%, which was validated by the rate reported by Rey and Brenner (2016). The trend presented by the results of the stock of ERA using the three approaches described in **Figure 2** reveals an increase in the first half of the 21st century and a flattening in the second half (**Figure 5**). The comparison of ERA results with previous studies shows a good fit.

The evolution of direct final energy consumption according to the baseline scenario shows a trend with three phases: (1) an increase until 1990, (2) stagnation for the period 1990–2010 and (3) a decrease from 2010 onward (**Figure 6**). Emissions results depict a rapid decrease until 2025, and a slower decrease until 2100. Historical energy and emissions results fit well with the overall trend presented by the statistical data; however, they fail to capture the annual data fluctuations, which might be caused by annual climatic variability. These fluctuations were quantified to differ from model results by ±12% for historical years; therefore, future energy consumption and emissions are expected to lie

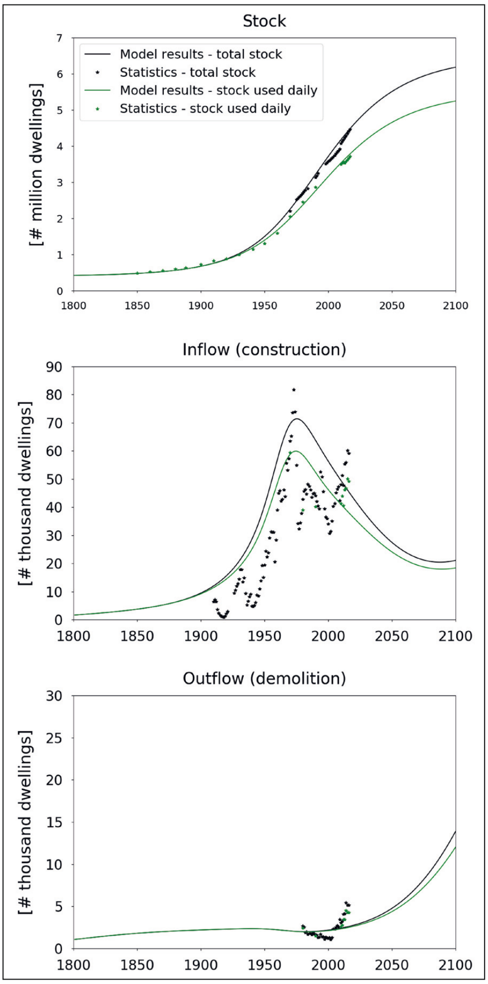

Figure 4: Evolution of the stock, inflow and outflow for the total stock and stock used daily for the period 1800–2100, for the baseline scenario. The model results are compared with statistical data.
Sources: FSO (2018a, 2019a, 2019b).

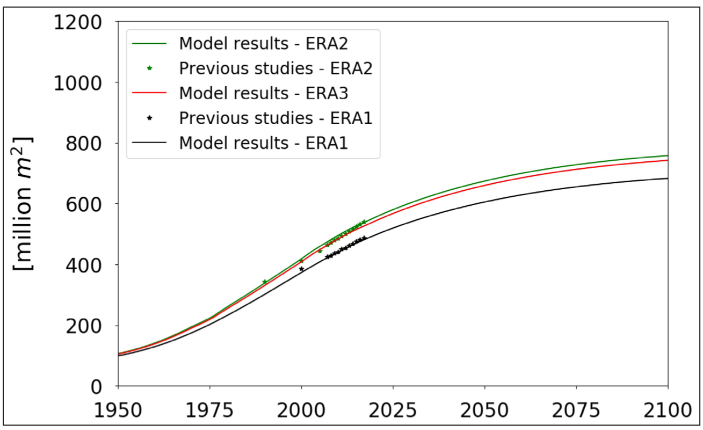

Figure 5: Stock of energy reference area (ERA) using three calculation approaches (described in Figure 2). Historical results are compared with previous studies (SFOE 2018a, Siller *et al.* 2007; Wallbaum *et al.* 2009). Future results correspond to the baseline scenario.

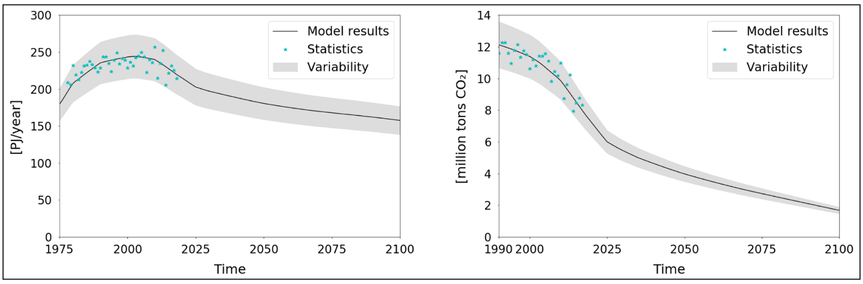

Figure 6: Evolution of direct final energy consumption and direct CO_2 emissions associated with the use phase of Swiss residential buildings for the baseline scenario, including the variability range due to annual fluctuations. The model results are compared with statistical data (FOEN 2019b; SFOE 2019).

Table 2: Relative sensitivities in 2020 with +10% of input parameter.

Parameters	Energy results	Emissions results
Lifetime	–0.02	–0.02
Renovation cycle length	0.33	0.39
Realised renovations	–0.21	–0.25
Occupancy factor	0.09	0.09
Energy intensity SH R1	0.39	0.47
Energy intensity DHW R1	0.09	0.11
Energy intensity Others R1, R2	0.18	0
Energy intensity SH R2	0.27	0.32
Energy intensity DHW R2	0.02	0.03

Note: Negative values indicate that the parameter increase leads to an output decrease.

within this range. Similarly, energy consumption segmented by energy carrier presents a good fit with the overall statistical trends (see Appendix F in the supplemental data online).

The results in **Figure 6** were obtained using ERA3 and accounting for user behaviour (real energy). Energy results using ERA1–2 and not accounting for user behaviour (technical energy) were computed to study potential discrepancies and to compare the results with previous studies (see Appendix F in the supplemental data online). Energy results using different ERA approaches lead to differences of 10% in 2050. Historical results obtained using the same ERA approach are comparable among studies (Siller *et al.* 2007; Wallbaum *et al.* 2009). The results obtained accounting for user behaviour present about 20% higher real energy consumption in 2050 compared with technical energy, which is in line with the results of Schneider *et al.* (2017). The scenario analysis was conducted using ERA3 and real energy consumption because they account for user behaviour, occupancy in holiday houses and provided the best fit to statistical data.

The results of the SA for 2020 reveal relative sensitivities < 0.5 (**Table 2**), which highlights that the historical energy and emissions results are not very sensitive to changes in highly uncertain parameters. The SA results for 2050 show large differences in the impacts of parameters; however, most relative sensitivities are < 0.5, which indicates that the model is not very sensitive to changes in the future input data of parameters. The parameters with relative sensitivities > 0.5 are population, people per dwelling, correction factor and user behaviour (see Appendix F in the supplemental data online). The impacts of population, FApC (determined by people per dwelling and floor area per dwelling) and correction factor are expected to be high given that they determine the stock (living area and ERA), which is the driver of the model. The user behaviour shows a coefficient for energy results of about 0.57, which is similar to that reported by Sandberg *et al.* (2017) using a similar model formulation. The parameters with sensitivities > 0.5 are included in the scenario analysis, except for population, for which the medium projection for all scenarios was assumed. The future evolution of population is highly dependent on economic developments as well as migration and fertility policies, which are outside the scope of this study.

Given the results of the uncertainty analysis, the model was regarded as robust and suitable for scenario analysis.

3.2 Scenario analysis

The scenario analysis for both direct final energy consumption and direct CO_2 emissions shows that all scenarios comply with the Kyoto Protocol and the first intermediate goal of the ES2050, given that these goals are defined for 2020, which is considered as the current year (**Figure 7**).

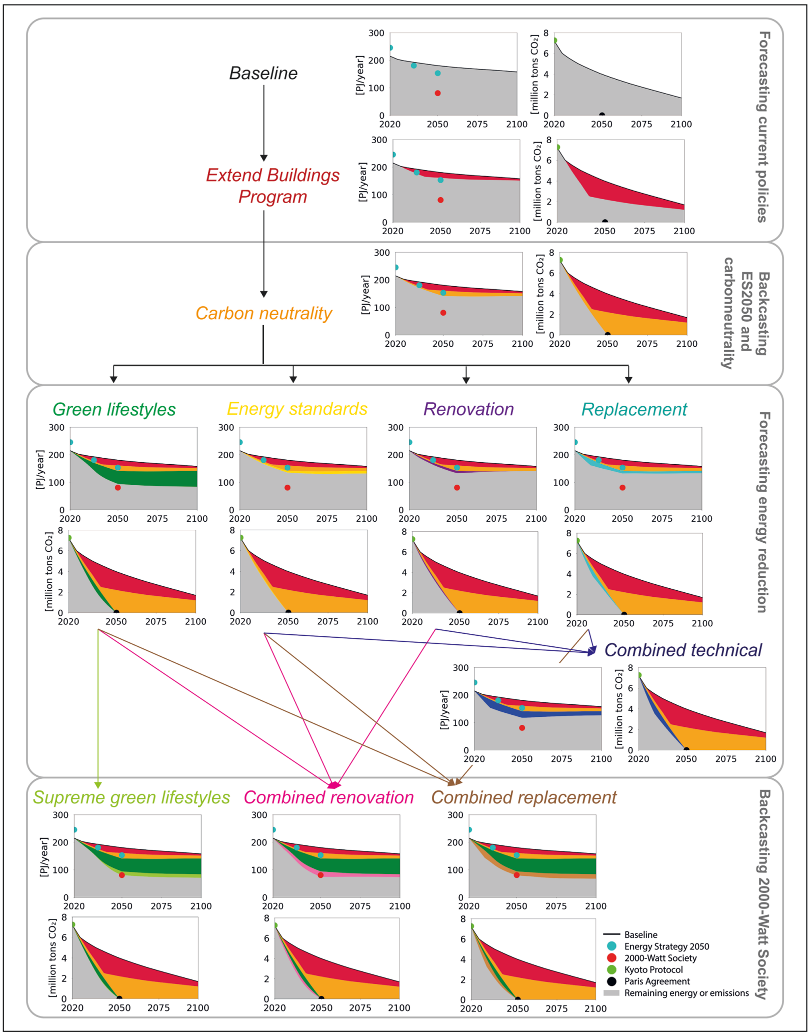

Figure 7: Direct final energy consumption and direct CO_2 emissions pathways associated with the use phase of Swiss residential buildings for 11 scenarios and compared with the Kyoto Protocol, Paris Agreement, ES2050 and 2000-Watt Society goals. The energy and emissions savings are segmented according to the premises of the scenarios.

The future evolution of energy consumption and emissions triggered by assuming that current policies are in place (baseline) is insufficient to fulfil any of the goals beyond 2020. The trend shift observed in 2025 corresponds to the termination of the BP. An extension of current policies (extend Buildings Program) leads to 11% and 45% reductions in 2050 for energy and emissions, respectively, compared with baseline, which are insufficient to satisfy the goals for 2050. The shift observed in the emission trend in 2040 is triggered by the complete disappearance of oil heaters.

Extending the BP together with a rapid and gradual phase-out of fossil fuels until 2050 (carbon neutrality) results in a stock consuming about 22% less energy compared with baseline and emitting zero emissions in 2050. The carbon-neutrality scenario complies with the ES2050 and Paris Agreement goals, but not with the 2000-Watt Society goal. This scenario requires a twofold increase of energy supplied by renewable energies and heat pumps in 2050 compared with the baseline (**Figure 8**), and it leads to a 30% reduction of cumulative CO_2 emissions by 2050 compared with the baseline (**Figure 9**).

Compared with the baseline, the green lifestyles, energy standards, renovation, replacement and combined technical scenarios lead to energy savings of 48%, 25%, 26%, 27% and 35%, respectively. Despite the energy reductions mentioned, none of the scenarios reaches the 2000-Watt Society goal. The replacement and combined technical scenarios trigger a 34 times higher demolition and a 3.4 times higher construction during the leaching phase compared with the baseline, in order to preserve the stock (see Appendix G in the supplemental data online). After the leaching phase, the demolition and construction activities are lower compared with the baseline, given that the stock is younger.

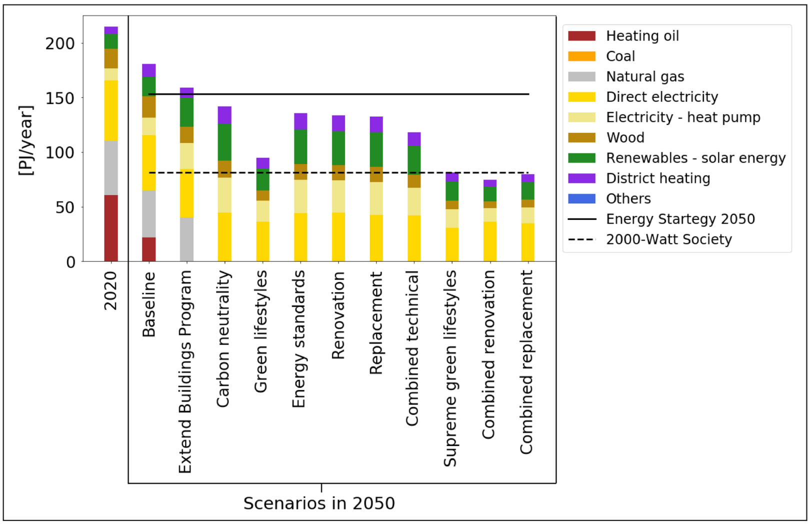

Figure 8: Direct final energy consumption for the use phase of Swiss residential buildings segmented by energy carriers in 2020, and in 2050 for the 11 scenarios compared with the ES2050 and the 2000-Watt Society goals.

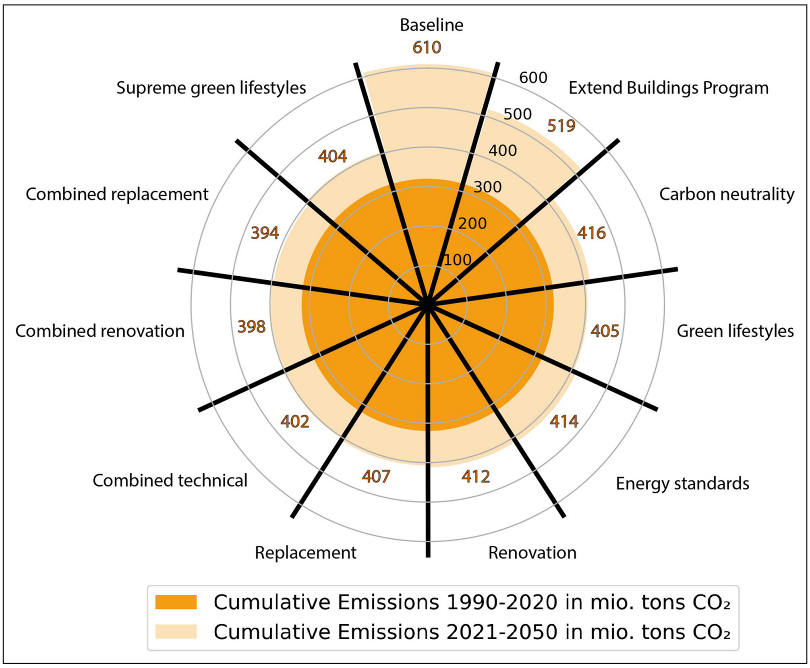

Figure 9: Cumulative CO_2 emitted during the periods 1990–2020 and 2021–50 for all scenarios. The exact value for the entire time period is provided for each scenario.

The 2000-Watt Society goal can be met by three alternative scenarios: supreme green lifestyles, combined renovation and combined replacement. The three scenarios lead to energy pathways with a reduction of about 55% in 2050 compared with the baseline. The energy supplied by renewable energies and heat pumps is reduced by 54% and 55%, respectively, in 2050 compared with the carbon-neutrality scenario. For the three scenarios, a substantial reduction in SH demand is observed, which makes other uses (electric appliances, ventilation, air-conditioning and minor uses) a dominant energy use in 2050 (see Appendix G in the supplemental data online). The combined replacement scenario triggers the same construction and demolition results as in the replacement and combined technical scenarios. The supreme green lifestyles scenario leads to a reduction in construction of about 75% in 2050 compared with the baseline. The combined replacement scenario provides the lowest cumulative CO_2 emissions, followed by the combined renovation and supreme green lifestyles scenarios; however, the differences are small.

4. Discussion

4.1 Uncertainties and limitations

While building stock models have been used extensively to study building stock dynamics (Bergsdal *et al.* 2007; Müller 2006; Stengel 2014), they are limited by input data, model assumptions and scope. The two SA found that the model is not very sensitive to changes in the historical input data of highly uncertain parameters and to changes in the future input data of parameters. However, the highest sensitivities for 2020 were found for parameters related to renovation activities and technical energy consumption in buildings, which reveals that higher data quality for these parameters could improve the model. The highest sensitivities for 2050 were found for lifestyle-related parameters, which highlights the importance of including them in long-term scenario analyses. The limitations related to model assumptions and scope are summarised as follows and explained in detailed below: (1) a constant lifetime for cohorts and types, (2) average energy intensities define cohorts and types, (3) user behaviour depends on technical energy consumption in buildings, (4) the outdoor climate remains constant, (5) unclear boundaries between residential and non-residential stock and (6) energy consumption and emissions associated with construction, demolition, energy and material production activities are disregarded.

Lifetimes of buildings and demolition activities are still poorly understood. Following previous research (Vásquez *et al.* 2016), demolition activity was modelled as a function of a normally distributed constant lifetime for all cohorts and types; however, drivers such as land price, rents, cultural heritage and households' preferences influence demolition activities, and these drivers were considered to be outside the scope of this study. The non-inclusion of such drivers might explain the short-term fluctuations in construction and demolition not captured by the model results. While this behaviour is typical of stock-driven models, these models are robust in portraying long-term dynamics (Müller 2006).

The model formulation considers cohorts and types which are defined by average energy intensities. This approach captures the heterogeneity of the stock; however, it fails to capture the variability within a specific cohort and typology. Considering normally distributed averages could reflect the variability, but would be conditioned to the availability of disaggregated data.

User behaviour was considered to depend on the technical energy intensity of buildings. While this approach has been used in previous publications (Sandberg *et al.* 2017) and offers a first attempt to account for user behaviour, it simplifies the drivers by excluding the purchasing power and lifestyle preferences of households, and it might include uncertainties associated with the technical energy intensity in user behaviour. This highlights the need for more comprehensive approaches to model user behaviour, which is especially important in long-term analyses.

The outdoor climate was assumed constant at today's climate; however, previous research for Switzerland showed that global warming could cause a 10–40% decrease in SH and a 250–1300% increase in cooling by the end of the century compared with 1980 (Berger & Worlitschek 2019; Christenson *et al.* 2006). Given that about 60% of SH demand was supplied by fossil fuels in 2017, a decrease in SH could assist the transition toward carbon neutrality. The increase in cooling could substantially increase electricity demand, and thus condition the supply of a carbon-free electricity mix.

The boundaries between residential and non-residential stock are subject to national definitions and reporting procedures. Accordingly, FApC was calculated and used to obtain the residential stock; however, the boundary between residential and non-residential floor areas in buildings sharing different functionalities or in buildings undergoing functionality conversions are often not clearly reflected in the statistical data. More systematic statistical reporting procedures could help to refine the modelling exercise.

Energy consumption and emissions associated with construction, demolition, energy and material production activities (embodied emissions) are disregarded; however, the potential indirect environmental impacts of the scenarios are discussed in section 4.3. These activities could be accounted for by expanding the system definition to include them as processes. A simple approach to include indirect emissions associated with the production of electricity and district heating is to account for their carbon intensities. When such accounting is conducted using the values from Mavromatidis *et al.* (2016), the emissions results for 2010 are 3% higher than shown in **Figure 6**.

While the limitations highlight possible further developments, the results of the uncertainty analysis show that the model is robust.

4.2 Modelling disruptive measures

As part of the scenario analysis, the authors modelled a disruptive measure triggering an increased replacement of the most energy-consuming buildings by highly energy-efficient buildings with a combined lifetime-leaching approach. The results obtained using the combined approach show that the method captures both the heterogeneity of the stock and the complete demolition and replacement of the targeted segment of the stock (see Appendix G in the supplemental data online).

This study considered a leaching rate leading to the complete demolition of the non-renovated buildings built before 1990 during the leaching period 2021–30. Such a definition was set on purpose as a radical intervention in order to study the effects of disruptive measures. However, the definition of the leaching is flexible and thus it could be defined using other rates, segments of the stock and leaching periods. Despite the flexibility of the combined approach, it is subject to the limitations exposed in section 4.1. The combined approach has the potential to model other disruptive phenomena in building stocks such as wars and natural disasters (*e.g.* flooding, earthquakes, fire events), and it could be applied in other sectors such as transportation to model car accidents in the vehicle fleet.

4.3 Policy implications

The scenario analysis indicates that the main leverage points for energy savings during the use phase of Swiss residential buildings reside in lifestyle changes, whereas emission reductions can be highly levered by technological developments.

In terms of emissions goals, the Paris Agreement can be achieved by extending current policies together with a rapid replacement of fossil-fuel heaters by heat pumps and renewable energies, leading to their complete replacement by 2050 (carbon neutrality). These measures require high economic investments to extend current policies (BP beyond 2025) and to promote the rapid replacement of fossil fuel heaters. The carbon neutrality scenario triggers an increase in electricity and renewable energy demand, which could condition the feasibility of reaching carbon neutrality in all sectors by shifting the burden to the energy supply sector. This burden could be eased by reducing energy demand, which could also lower cumulative CO_2 emissions and thereby expedite efforts to remain within the carbon budget.

In terms of energy goals, while the ES2050 can be met by the technological developments presented above, the 2000-Watt Society target can only be reached if lifestyle changes are considered, as shown by the combined technical scenario, where a set of ambitious technological developments is insufficient to reach the target. The highest leverage of lifestyle changes lies in lower indoor temperatures and heating only dwelling areas, which, combined with high energy standards and either higher renovation rates or replacement measures, could provide energy savings sufficient to reach the 2000-Watt Society target, as shown by the combined renovation and combined replacement scenarios. These two scenarios require high economic incentives to promote Minergie-A and Minergie-P standards for new and renovated buildings, respectively, and either a renovation rate of 3% or the replacement of buildings consuming > 140 kWh/m^2/yr. The replacement measure might induce social reluctance in households living in the targeted buildings because they need to move to other dwellings temporarily. Both scenarios require lifestyle changes toward optimisation and the responsible use of SH to minimise the performance gap of buildings and thus reduce the rebound effect of overheating due to energy-efficiency gains. Such optimisation could be assisted by temperature-controlling systems (Khoury *et al.* 2017), which could be promoted via economic subsidies.

Complementing the above-mentioned lifestyle changes with a 15% lower FApC and construction gradually dominated by MFH could be an alternative lifestyle-based strategy to meet the 2000-Watt Society target (supreme green lifestyles). As suggested by Drouilles *et al.* (2017), policies supporting such scenario are difficult; however, the promotion of densification in new buildings or extensions and reorganisations in SFH could help. The scenarios meeting the 2000-Watt Society target re-emphasise the findings of the SA for 2050 regarding the importance of including lifestyle aspects in long-term scenario modelling and policy discussions.

The strategies for meeting the 2000-Watt Society target have substantial impacts on construction and demolition activities. The combined replacement scenario leads to an increase in construction and thus a potential increase in material production activities, which might result in an increase of indirect energy and emissions. Similar effects are expected in the combined renovation scenario due to a substantial increase in renovation activity. Müller *et al.* (2013) found that greenhouse gas emissions associated with material production for construction can be critical for reaching the global climate targets. The supreme green lifestyles scenario leads to lower construction activity and thus a potential decrease in indirect environmental impacts.

5. Conclusions

This study presented 11 scenarios triggering different pathways for direct energy consumption and direct CO_2 emissions associated with the use phase of Swiss residential buildings. The scenario analysis indicates that the main leverage points for reducing energy reside in lifestyle changes, such as lower indoor temperatures, whereas emission reductions can be highly levered by technological developments. Reaching the Paris Agreement, ES2050 and 2000-Watt Society goals is possible, but ambitious strategies are needed. This study provides a first assessment of disruptive measures and expands the analysis of lifestyle changes, thereby setting the grounds for enlarging the current portfolio of Swiss climate change mitigation strategies for the residential building sector. Given that the strategies are highly ambitious, more research is needed to evaluate economic and social aspects. Further research is also needed to quantify the effects of the strategies on indirect energy and emissions associated with buildings, and to study the options for reducing carbon emissions in materials production through material choice, production technologies, reuse of components and recycling. The model presented can be used as a backbone for such system expansion, eventually enabling a simultaneous evaluation of climate change mitigation and circular economy strategies.

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Competing interests

The authors have no competing interests to declare.

Data accessibility

The model developed within this work and the input data are available at https://zenodo.org/record/3984758#.XzZBsegzZaQ.

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Supplemental data

Supplemental data containing Appendices A–F, the model description, a detailed description of the parameter estimation and uncertainty analysis, and additional model results can be accessed at DOI: https://doi.org/10.5334/bc.61.s1

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