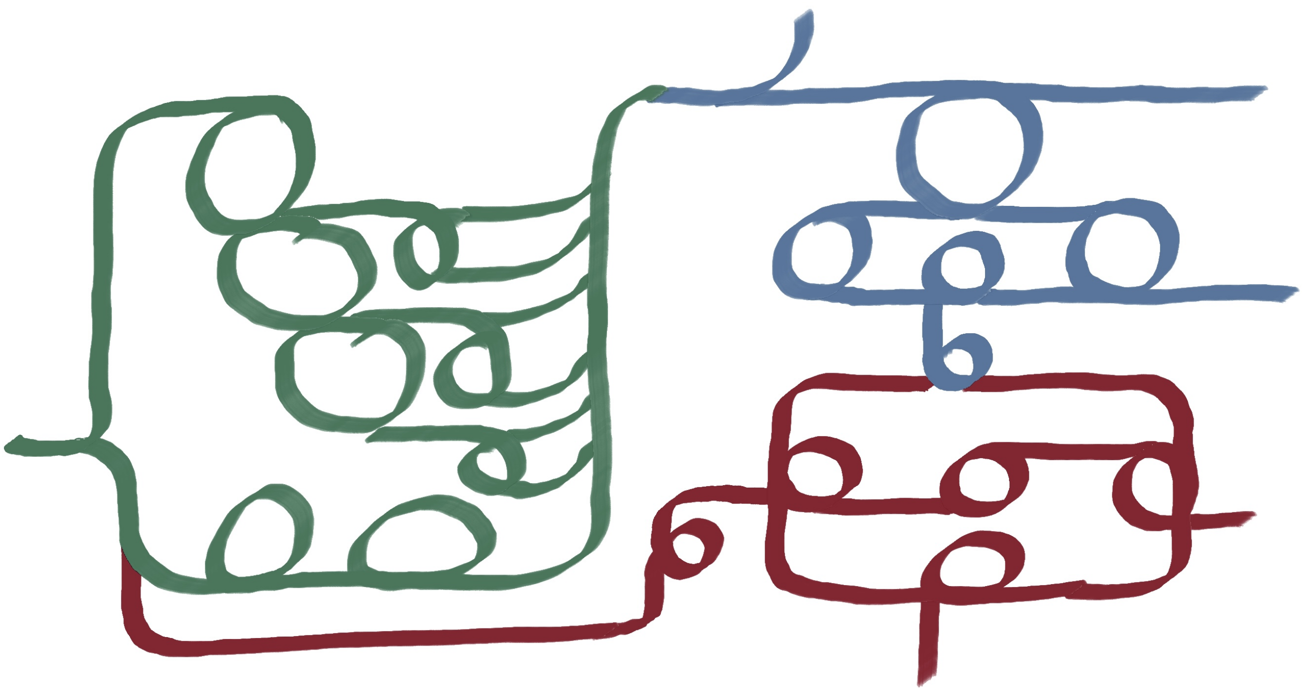
Integrating Reuse in MaTrace Models

An implementation and evaluation

Raphael Andreas Elbing



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Summary

The growing wold population gaining affluence is driving the extraction of raw materials. Resource availability is finite and concerns about future supply shortages rise. An approach to tackle this problem is circular economy which entails multiple strategies to reduce the demand of virgin materials. The implementation of those strategies require knowledge about material stocks and flows in a society. Material Flow Analysis can provide those insights. This fast developing field brought about MaTrace models which allow to trace the fate of materials in an open-loop recycling system. Recycling is only one of multiple circular strategies, thus the purpose of this research is to integrate an elaborate reuse model into a MaTrace model to build the foundation of a model which considers multiple circular strategies in sufficient ways.

Two existing models were combined to achieve this: Consumer goods present in the MaTrace model were redirected into a reuse model and the end of life products of the reuse model were fed back into the MaTrace model. The impacts of this model extension were investigated by comparing the total in-use stock when considering one, two, and three consumer products' use cycles. Furthermore, Monte Carlo simulations were conducted to gain an understanding of the model behaviour.

The results show that the total in-use stock increases in the peak by 8 % when reuse is considered. However, the gross stock dynamics do not change significantly in comparison to the original model. The evaluation of the Monte Carlo simulations revealed that the input which contributes the most uncertainty to the total in-use stock is the split of the initial material inflow. Furthermore, the results of the Monte Carlo simulations appear to be strongly connected to the initial input data. On the basis of this research it can be recommended to further extend MaTrace models to obtain a more comprehensive representation of a circular economy. Furthermore, MaTrace models using time series data for inflows and model parameter have to be created, this way MaTrace models can follow the evolution of MFA from static to dynamic models.

Contents

Nomenclature

Abbreviations

Abbreviation	Definition
CRM	Critical raw material
DQR	Data Quality Rating
DRC	Democratic Republic of Congo
EE	Electronic equipment
EOL	End-of-life
ETM	Energy transition metal
EV	Electric vehicles
GDP	Gross Domestic Product
GHG	Greehnhouse gas
IE	Industrial ecology
IOT	Internet of things
MFA	Material Flow Analysis

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Introduction

Throughout the current century raw material extraction constantly increases. A commonly known driver is a growing, more affluent world population which rises concerns about future resource availability (Calvo et al., 2017). Moreover critical raw materials (CRM) as lithium or cobalt are subject to other drivers. The accelerating energy transition from a fossil fuel based system towards renewable energy sources requires enormous amounts of CRMs for production and storage. Although, there is currently no shortage in supply, the demand due to global climate ambition may exceed possible supply volumes (Pommeret et al., 2022). Additionally, the private use of portable electronics accelerates because of technological developments as internet of things (IOT) or 5G appliances (Desai, 2020) all adding to the demand of CRMs.

These mingled construct of demand and supply holds complex implications regarding sustainability. Looking at the ecological aspect of sustainability one finds that those materials are required to minimize the carbon emissions of the energy system on the one hand. On the other hand, the mining of some materials leads to environmental pollution (Sovacool, 2019). Regarding the social component of sustainability it is apparent that the implications of CRM mining are severe for some materials. Cobalt for example is mainly mined in the Democratic Republic of Congo (DRC) where insecure mining conditions lead to reoccurring human rights violations such as child labor (Sovacool, 2019). For those reasons it is highly relevant for the field of industrial ecology (IE) to study material demand, usage, and supply.

Since the usage of CRMs appears to be unavoidable, losses in production and waste management have to be minimized and resource efficiency has to be optimised. Resource efficiency is broadly defined as the value created by a resource input while also considering environmental impacts. The term resources as it is used in this research covers amongst others raw materials, energy, or water (Hirschnitz-Garbers et al., 2013). In the context of this thesis resources must be understood as the length and intensity of material usage in a system.

An elaborate concept on how to increase resource efficiency is circular economy. The concept entails a model of production and consumption with the target to reduce material waste by moving from a linear economy (take-make-consume-throw away) towards a circular economy (“Circular economy”, 2015). Multiple strategies can contribute to the transition into a circular economy. The 9R framework classifies those strategies.

Circular economy		Strategies	Description
	Smarter product use and manufacture	R0 Refuse	Make product redundant by abandoning its function or by offering the same function with a radically different product
		R1 Rethink	Make a product use more intensive (e.g. by sharing product)
		R2 Reduce	Increase efficiency in product manufacture or use by consuming Fewer natural resources and materials
	Extend lifespan of product and its parts	R3 Reuse	Reuse by another consumer of discarded product which is still in good condition and fulfils its original function
		R4 Repair	Repair and maintenance of defective product so it can be used with its original function
		R5 Refurbish	Restore an old product and bring it up to date
		R6 Remanufacture	Use parts of discarded product in a new product with the same function
		R7 Repurpose	Use discarded product or its parts in a new product with different function
	Useful application of materials	R8 Recycle	Process materials to obtain the same (high grade) or lower (low grade) quality
		R9 Recover	Incineration of material with energy recovery
Linear economy			

Table 1.1: 9R circular economy framework by Kirchherr et al. (2017). Strategies become less circular from top to bottom.

The Table 1.1 shows, that the framework lists strategies by their circularity. Refuse within the strategy cluster "Smarter product use and manufacture" is claimed to be the most effective one. Reuse makes the fourth place in the ranking within the cluster "Expend lifespan of product and its parts".

But rather than applying those strategies blindly it is important to gain an understanding about society's metabolism first. In this context, the method Material Flow Analysis (MFA) offers important insights since it aims to study and quantify material stocks and flows in defined regions and temporal scopes. The evolution of the method gained momentum in recent decades. MFA started out with static models which consider only the stocks and flows of one year. On this basis, dynamic MFA was developed which allows to model past material flows and stocks based on historical data but also future flows and stocks based on scenarios (Müller et al., 2014). Hence, the tool can offer insights on where to apply which strategy to reach a maximum improvement in resource efficiency.

A model variant which gained popularity over the last years is the MaTrace model. The models specialty is the ability to showcase losses in an open-loop recycling system. It shows the fate of the material by tracking the inflow of one specific year over the coming years (Nakamura et al., 2014, also see Section 1.1.2). But according to the 9R framework recycling is not the most effective strategy to increase resource efficiency. Multiple scholars integrated other strategies as reuse into the original MaTrace model (Klose & Pauliuk, 2021; Pauliuk et al., 2017; Zhang et al., 2021, also see Section 1.1.2). However, the integration or reuse in those models is rather simplistic and does not necessarily match the state of the art in reuse modeling in MFA (see Section 1.1.3).

Therefore, the main target of this master thesis is to integrate reuse in a more elaborate fashion into a MaTrace model and to evaluate its impact and uncertainties. The following chapter of this thesis provides a state of the art about the MaTrace modelling approach, the modelling of reuse, and a description of modeling uncertainties on the example of survival curves in dynamic Material Flow Analysis (MFA). Research gaps and research questions are derived based on this state of the art. This is followed by a brief introduction to the case study. The second chapter provides the methodology describing how existing models were used and how modelling approaches are simplified, followed by a chapter describing the used data. The results of the research are provided in the fourth chapter, followed by a discussion and a conclusion.

1.1. State of the art

1.1.1. Dynamic MFA and MaTrace models

Primary material production affects economy, society, and environment in various ways. Some metals are scarce (Godoy León et al., 2020) causing dependencies on suppliers who cannot ensure safe working condition and involve child labour as it is the case for cobalt (Sovacool, 2019). Moreover, primary material production leads to GHG emission and other negative environmental impacts (Pauliuk et al., 2017). Because of the economic and environmental relevance, it is important to gain more knowledge about anthropogenic material flows and cycles (Jarrín Jácome et al., 2021).

A commonly used tool which serves this purpose is Material Flow Analysis (MFA). The original model as introduced by Baccini and Brunner (1991) describes material stocks and flows in a region with the temporal scale of one year. Hence, those models represent a snapshot in time without considering any past or future developments. Therefore, one speaks about static MFA when referring to these models.

As described, knowing stock and flow dynamics is important since it provides insights to future resource use, production and waste management planning, and potential environmental problems (B. Müller, 2006). Motivated by these reasons B. Müller (2006) introduced dynamic stock modelling (Sartori et al., 2016) which builds the foundation of dynamic MFA. This method of stock and flow quantification allows for evaluation of model inputs present as time series by calculating the respective stocks and flows. A static MFA model always complies with the law of mass conservation. There are multiple characteristics to differentiate dynamic MFA models. A key characteristic describes whether the model is inflow- or stock-driven. The following figure shows, that there are three elements to be determined; the inflow I, the stock S, and the outflow O.

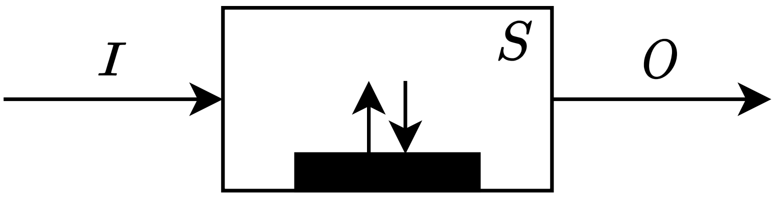

Figure 1.1: Single dynamic stock S with one inflow I and one outflow O

Stock driven models calculate I and O based on the stock S itself and a survival curve $s(t)$ (see Section 1.1.5 for more explanation on survival curves). In contrast, inflow driven models calculate the S and O based on the inflow I and the survival curve $s(t)$ (Müller et al., 2014). In the following, the calculations for an inflow-driven model as depicted in Figure 1.1 are presented. This concept will be used throughout this thesis. Assuming there is a data set consisting of an input series covering three years and a survival curve (see following table):

Time t and t'	Inflow $I(t)$	Survival curve $s(t')$
0	3	1
1	5	0.8
2	4	0.5

Table 1.2: Example data for inflow driven model

Then the inflow and the survival curve are exogenous model variables since they do not depend on any other variable in this case. The stock and the outflow are endogenous model variables since they depend on the model inputs (Müller et al., 2014). The stock can be calculated using the following formula (inspired by B. Müller, 2006):

$$S(t) = \sum_{\tau=t_0}^{t} I(\tau) \cdot s(t-\tau) \tag{1.1}$$

The outflow is then calculated via the net flow N:

$$N(t) = S(t) - S(t-1) \tag{1.2}$$

$$O(t) = I(t) - N(t) \tag{1.3}$$

When applied in a model, those calculations are executed via a cohort matrix. The following cohort matrix belongs to the data as presented in Table 1.2:

	0	1	2
0	3	0	0
1	2.4	5	0
2	1.5	4	4

Table 1.3: Example cohort matrix

Each column of the cohort matrix shows the depreciation of the inflow of one year (cohort) over time (rows). Since there is no stock depletion in the first year (see Table 1.2, survival curve $s(0) = 1$) the diagonal axis holds the inflow. With the help of those matrices the total stock S can be calculated by summing up the rows (for more information regarding the basic calculations see Lauinger et al. (2021)).

Besides the modeled system itself, and depending on whether a model is inflow- or stock-driven, models vary in their temporal scope (retrospective or prospective) and their regional scope (e.g., regional, national or global). Furthermore, some models consider hibernating stocks (also see Section 1.1.3).

Although dynamic MFA modelling might appear as straight forward, diverse approaches in extrapolating input data can be found as well. This is done to model the future or to test different scenarios which often rely on drivers. An example for this is the intensity-of-use hypothesis which assumes a relation between the demand of a material and the gross domestic product (GDP) of the region in focus. The review on dynamic MFA of Müller et al. (2014) found that extrapolation methods are often prone to over simplification, for example by not accounting for the scarcity of the material. Hence, interdisciplinarity is required in order to analyse society's metabolism (Lauinger et al., 2021). Dynamic MFA together with dynamic stock modelling forms the basis for MaTrace models. Its purposes and function will be described in the following section.

1.1.2. MaTrace model

Motivation and Purpose

The original MaTrace model of Nakamura et al. (2014) provides an elaborate model to track the fate of materials in an open-loop recycling system. This development is relevant since recycling is a key strategy to reduce the dependency on virgin materials. Therefore, it is essential to understand the basics about it.

Recycling has the potential to bring about closed material cycles requiring only little primary material input. If recycling is in place, the virgin material input depends on the following three factors: The growth rate of the in-use stocks, the ability of waste management facilities to recover a scrap and the ability of recycling companies to produce high quality secondary material while maintaining a high material efficiency (Pauliuk et al., 2017). Besides those factors, recycling can be functional or non functional. Materials recovered in functional recycling are fit to be reused for the same high quality products while materials recovered in non functional recycling end up in low-end products or as contaminants in materials (Godoy León et al., 2020).

There are, furthermore, factors concerning the actors participating in the use phase which determine the amount of material entering recycling. This depends on the lifetime of products on the one hand (see Section 1.1.3) and on the other hand on the waste separation performance of actors. How well actors separate waste is determined by their knowledge and perception of waste management (Uhunamure et al., 2021). Minimizing the described losses in recycling is the target of sustainable management and circular economy strategies. To do so, knowledge about the pathway of materials in an open-loop recycling system are required. The original MaTrace model by Nakamura et al. (2014) aims to fill this knowledge gap. It is able to trace the fate of materials which entered the system at beginning of the regarded period. This way the quantity of losses, functional and non functional recycling become apparent (Nakamura et al., 2014). It is important to understand that the model only considers *one cohort*, the virgin material input of only one year. It then traces the whereabouts of this single input over time.

How it works

The precise structure of a MaTrace model varies insignificantly depending on application and scope. Therefore, the fundamental functionalities are explained based on a generic model as displayed in Figure 1.2 clustering the elements into Use, End-of-Life, and Production following Godoy León et al. (2020).

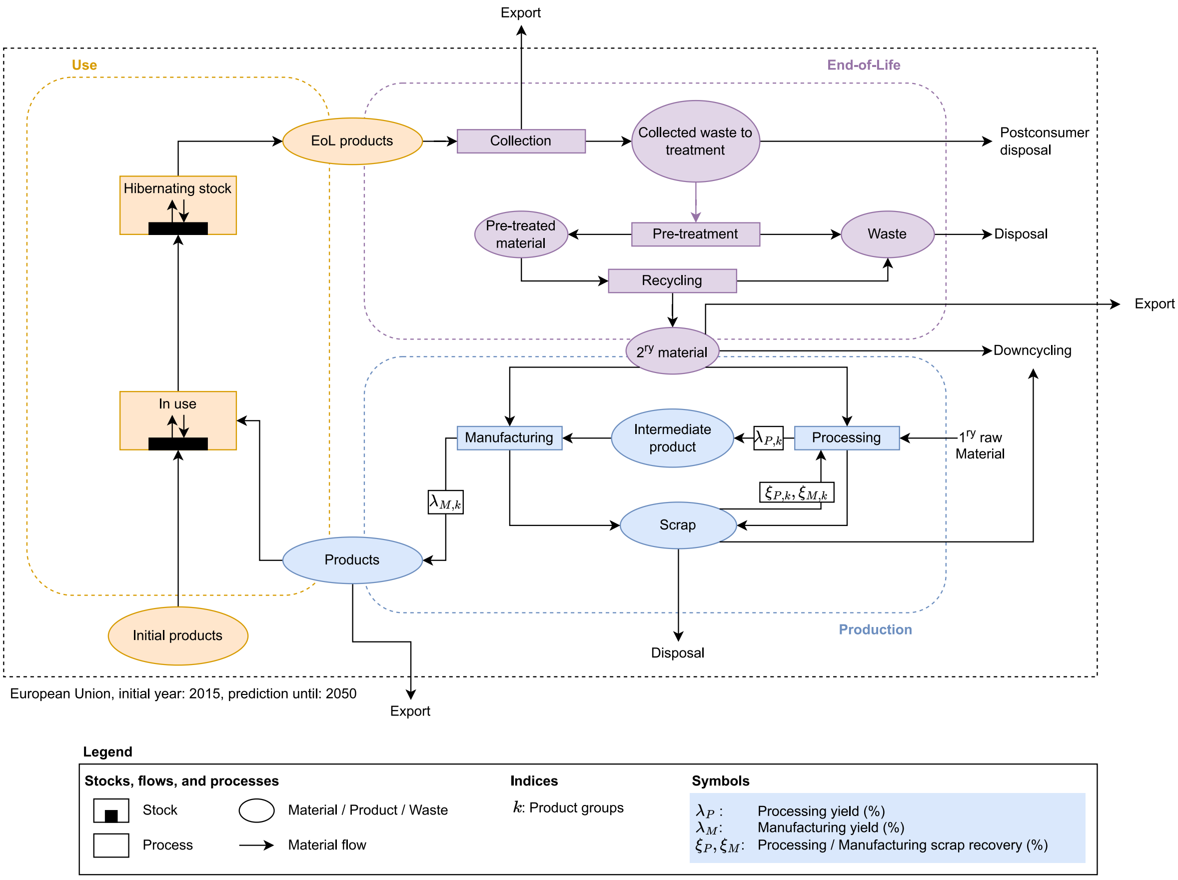

Figure 1.2: Simplified MaTrace system diagram inspired by Nakamura et al. (2014) and Godoy León et al. (2020)

MaTrace models allow to track the whereabouts of a specific material entering the system at the beginning of the regarded period (one cohort, see Figure 1.2; initial products) across products and time. Hence, only one inflow, the initial product distribution, has to be provided. The initial products vector is summed up to 1 (or 100%) since MaTrace models trace the whereabouts of material in percent (Godoy León et al., 2020; Nakamura et al., 2014; Pauliuk et al., 2017; Zhang et al., 2021). The depletion of the initial stock is defined by distributions. Each product category has its own survival curve defined by multiple parameters depending on the distribution. This stock depletion defines the yearly outflow of End-of-Life products (Godoy León et al., 2020; Nakamura et al., 2014).

The processes in the End-of-Life and Production cluster are defined by process yields (efficiencies). Applying the principle of mass conservation, all flows are found. Outflows can also be exports or more specific losses than those presented in Figure 1.2. Furthermore, two allocation matrices were used. One allocating the shares of the products to different recycling processes and one allocating the secondary material to production processes (here manufacturing and processing) (Godoy León et al., 2020).

Other challenges posed in solving this system are the closed loops between *Manufacturing*, *Scrap*, and *Processing*. Once these loops are mathematically formalized, one finds an infinite geometric series. The following equation shows the series for the total outflow of produced products of the node *Manufacturing* x_k in the year t, where k is the index referring to the different product categories. $p_{Ml,k}$ is the product outflow of one round of recycling where l indexes the round (Godoy León et al., 2020):

$$x_k(t) = p_{M1,k} + p_{M2,k} + p_{M3,k} + \cdots \tag{1.4}$$

To solve this, an expression for the share of recovered scrap in recycling round one needs to be found first. Here $\xi_{P,k}$ indicates the processing scrap recovery, $\xi_{M,k}$ indicates the manufacturing scrap recovery, $\lambda_{P,k}$ represents the yield of the processing node, and $\lambda_{M,k}$ represents the yield of the manufacturing node (Godoy León et al., 2020):

$$N_k = \xi_{P,k} \cdot (1 - \lambda_{P,k}) + \xi_{M,k} \cdot (1 - \lambda_{M,k}) \cdot \lambda_{P,k} \tag{1.5}$$

Using N_k, $\lambda_k = \lambda_{P,k} \cdot \lambda_{M,k}$, and $m_k(t)$ which is the amount of refined materials being available for manufacturing one finds the following infinite geometrical series (Godoy León et al., 2020):

$$x_k(t) = \lambda_k \cdot (1 + N_k + N_k^2 + \cdots) \cdot m_k(t) \tag{1.6}$$

This series can be solved analytically (Weisstein, 2022) resulting in (Godoy León et al., 2020):

$$x_k(t) = \lambda_k \cdot (1 - N_k)^{-1} \cdot m_k(t) \tag{1.7}$$

This solution makes the system computable. A full derivation of the expression can be found in either the supporting information of Nakamura et al. (2014) or Godoy León et al. (2020).

Once the whole cycle is computed, the produced goods (equation above) flow back into the use stock and the cycle has to be repeated for each year in the considered time frame (also see Section 2.2). In every iteration the stock depletion of each previous cohort must be considered. This way the fate of the virgin material input of one year is tracked over multiple life- or recycling cycles. Hence, MaTrace does not evaluate the whole material present in the system but only the share which entered the system in one specific year.

Versions

Since the publication of the MaTrace model by Godoy León et al. (2020) of Nakamura et al. (2014), multiple further publications applied or extended the model (Scopus search with search term "MaTrace"). Only Takeyama et al. (2016) left the original model untouched while Godoy León et al. (2020) and Jarrín Jácome et al. (2021) adopted the model to suit the regarded material. Larger changes were implemented by Pauliuk et al. (2017) who developed a global MaTrace model, by Helbig et al. (2022) who traced multiple materials, and by Nakamura et al. (2017) who extended the model to trace the fate of substances in alloys.

Moreover, multiple publications implement circular practices as re-manufacturing (Zhang et al., 2021) and reuse (Klose & Pauliuk, 2021; Pauliuk et al., 2017; Zhang et al., 2019). Pauliuk et al. (2017) treat reuse as a byproduct of the global MaTrace model. A share of the end-of-life products of one region may enter the use phase of another region via trade. An altered lifetime of reused products is not considered.

Klose and Pauliuk (2021) explicitly treat reuse in their model by considering shares of end-of-life products which are reused. However, the considered lifetimes originate from durability standards or product warranty laws. It is explicitly stated that the lifetime of products entering the use phase does not change for reused products and throughout time.

Zhang et al. (2021) investigate the impact of the reuse of automotive engines. As for the examples above, they do not consider a decay in lifetime if an engine is reused but assume that a reused engine has the same lifetime as a new one.

Hence, the models considering reuse do so, by redirecting product flows without considering decays in lifetime, hoarding times, or the impact of consumer behaviour. This can pose an oversimplification which emphasizes the need for models representing circular strategies more realistically. However, Godoy León et al. (2020) first introduced hibernating stocks in their MaTrace model shifting the perspective on material efficiency towards the user.

What can be understood as MaTrace model

Based on the large variety of present MaTrace models it appears to be legitimate to extend existing once without loosing the label. All present models have in common that they consist of three major clusters: Use, End-of-life, and production. The consideration and calculation of the closed loop in the production cluster is the aspect which clearly distinguishes MaTrace from former dynamic MFA models. Furthermore, they all trace the whereabouts of only one initial material input. In this context, dynamic stock modelling is used to consider multiple life-cycles of one inflow (one cohort) (also see Section 2.2) and not a time series input as commonly used in dynamic MFA.

I deem the way reuse is considered in MaTrace models as insufficient. Thus, the current state or the art in modeling reuse will be explained in the following section.

1.1.3. Modeling reuse

Although reuse is not the leading strategy according to the 9R framework, it is highly relevant to investigate its impact since the markets for second-hand an refurbished goods have been growing steadily in recent years (Kwarteng et al., 2018). It is a valid strategy because service lifetime and resource efficiency are closely connected. A longer lifetime increases the usage of a spent resource which increases the resource efficiency of this very item. Therefore, it is highly relevant to understand when a service life ends. Quantifying lifetimes is especially difficult for consumer goods because consumers have individual motivations to discard products. This decision can be either driven by diminished product integrity or by obsolescence (den Hollander et al., 2017). In general, a use cycle ends with the obsolescence of a product, meaning the product lost its perceived value to its owner (Box, 1983).

It is crucial to understand that there are multiple ways a product can become obsolete to its owner. The most intuitive one is functional obsolescence, meaning the product lost its functionality (Glöser-Chahoud et al., 2019). In this context it needs to considered that a loss of functionality/performance did not necessarily occur but might be perceived by the user for other reasons (Makov & Fitzpatrick, 2021). Furthermore, the actual time span within which a product stays functional can depend on the users behaviour. Batteries for example have an expected lifetime of three to five years, their actual lifetime depends on the charging habits of the user (Beaulieu, 2021).

Planned obsolescence is closely connected to functional obsolescence. Planed obsolescence is a loss of functionality by design caused for example by software updates (Glöser-Chahoud et al., 2019). Besides its functionality, it is possible that a product stops to fulfill the requirements of the owner. In this case aesthetic obsolescence describes products which are perceived outmoded, psychological obsolescence covers products which are out of fashion (Burns, 2010), and technological obsolescence describes technologies which are supplanted by superior technology (Glöser-Chahoud et al., 2019). Besides individual particularities the social environment can have an impact on the decision to discard a product. Social obsolescence describes products becoming obsolete due to laws, regulations, or stigmatization (Burns, 2010).

On this basis it can be concluded that obsolescence and service lifetimes are highly user dependent. As a consequence, it was discovered that a product may be perceived as obsolete by one user but not by another which forms the basis for reuse. Hence, a product can go through multiple use cycles which would improve the resource efficiency of this particular item.

A phenomena preventing products from entering another use cycle or waste treatment is called hibernation, meaning the storage of obsolete but functional items by the consumer (Oswald & Reller, 2011). Hibernating stocks impair resource efficiency in two ways. Firstly, items appear to be stored for a long time. Wilson et al. (2017) found that the hibernation phase of mobile phones in the UK is almost three times longer than the use phase. Hence, resources in those item are not used during this time. Secondly, due to long storage periods products are more likely to become obsolete to other potential users. This diminishes the probability for product to enter another use cycle (Glöser-Chahoud et al., 2019).

Considering the inconsistent behaviour of consumer regarding obsolescence and hoarding times it becomes obvious that service lifetimes, hibernating stocks and reuse are hard to quantify and consequently hard to model. Obtaining needed data requires conducting surveys and interviews. Modeling reuse poses an interface from classical MFA to social science and showcases the interdisciplinarity which is required to quantify material flows in societies metabolism.

1.1.4. The reuse model

Material flows are usually modeled based on stock data, sales and estimated product lifetime. Due to the described phenomena of obsolescence, hibernating stocks and reuse create a discrepancy between high sales and low collection flows could be found.

Thiébaud et al. (2017) pointed out, that the following publications treated aspects of this issue. Williams et al. (2005) investigated the hoarding times of computers, Polák and Drápalová (2012) found hoarding times for mobile phone and Milovantseva and Saphores (2012) and Saphores et al. (2009) estimated the hoarded e-waste in households in the USA. Chung et al. (2011) estimated the storage time and amounts of among others computers, televisions, and washing machines in Hong Kong. Reuse and hibernation was also considered in multiple MFA studies (Parajuly et al., 2017; Steubing et al., 2009; Yoshida et al., 2009). However, Thiébaud et al. (2017) claim (to the best of their knowledge) that their model is the first dynamic MFA to distinguish between in-use, reuse, and hibernating stocks for electronic equipment (EE) while considering reuse and storage times.

The model itself (see Figure 1.3, in the following referred to as **reuse model**) is a cascading model considering three use and three hibernating stages where the third use and hibernating stage represent all further uses beyond (Thiébaud et al., 2017).

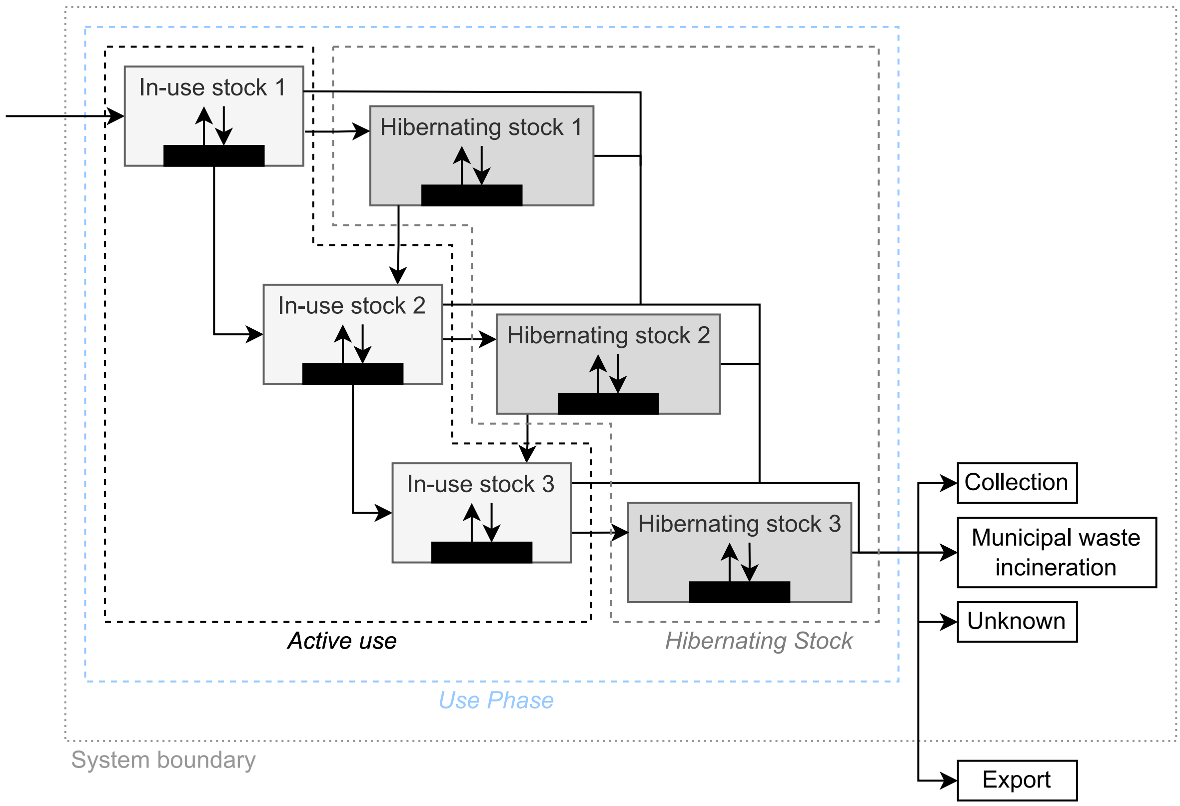

Figure 1.3: Reuse model system diagram by Thiébaud et al. (2017)

The original model as created by Thiébaud et al. (2017) is an inflow driven model considering multiple electronic devices. While the regional scope is clearly mentioned (Switzerland), a time frame to which the data is applicable is not provided. The model itself is a combination of multiple dynamic stocks which makes it a dynamic MFA model. Each of the stocks receives an inflow, a survival curve defines the stock decay and the outflow is distributed via transfer coefficients. Hence, the model requires extensive amount of data. Each product requires six survival curves (three for the use stocks and three for hibernating stocks) and 27 transfer coefficients to determine the fate of each outflow.

The required data is hard find thus the data was gathered in a separate publication. Thiébaud (-

Müller) et al. (2017) investigated the service lifetime, storage times, and disposal paths for ten electronic device types in Switzerland by conducting interviews and surveys. Their discussion of the results reflect the aforementioned factors contributing to uncertainty. Furthermore, it is mentioned that the data on reuse and disposal pathways might be object to subjective estimates. This limitation is in line with the results of another publication which investigated the difference in desired, expected, and actual measured lifetime. The study found that the actual measured lifetime is substantially smaller than the expected lifetime (Wieser & Tröger, 2015), this adds the dimension of consumer self perception and expectations.

Although, the model and the required data are subjected to deep uncertainty the introduced reuse model was found useful to understand alternations in consumer behaviour and use patterns (Glöser-Chahoud et al., 2019).

Since uncertainty will continue to be an important aspect of this work, the following section will clarify the uncertainties in dynamic MFA models inherent to survival curves.

1.1.5. Survival curves as example for uncertainties

Section 1.1.3 explained the underlying mechanisms causing consumer to discard product are extremely complex and non homogeneous. No matter the uncertainties, the end of life has to be represented in dynamic MFA modelling. To do so, the end of life of a whole basic population (e.g., a product group) is defined by the survival curve of a distribution. Miatto et al. (2017) showcased the difficulties and importance to select the right distribution by the example of buildings. The following explanation shall serve as an representative example for uncertainties in data and modeling choices in MFA modeling. Figure 1.4 displays the survival curves (A) and hazard rates (B) of the most commonly used distributions in MFA modelling. Survival curves represent the reliability of a product or a product group. In the context of MFA it represents the stock depletion of one single cohort (inflow into the stock at one point in time). Its value (y-axis) represents the share of material being in stock over time. The hazard rate represents the likelihood of an item failing (reaching its end of life) at a certain point in time.

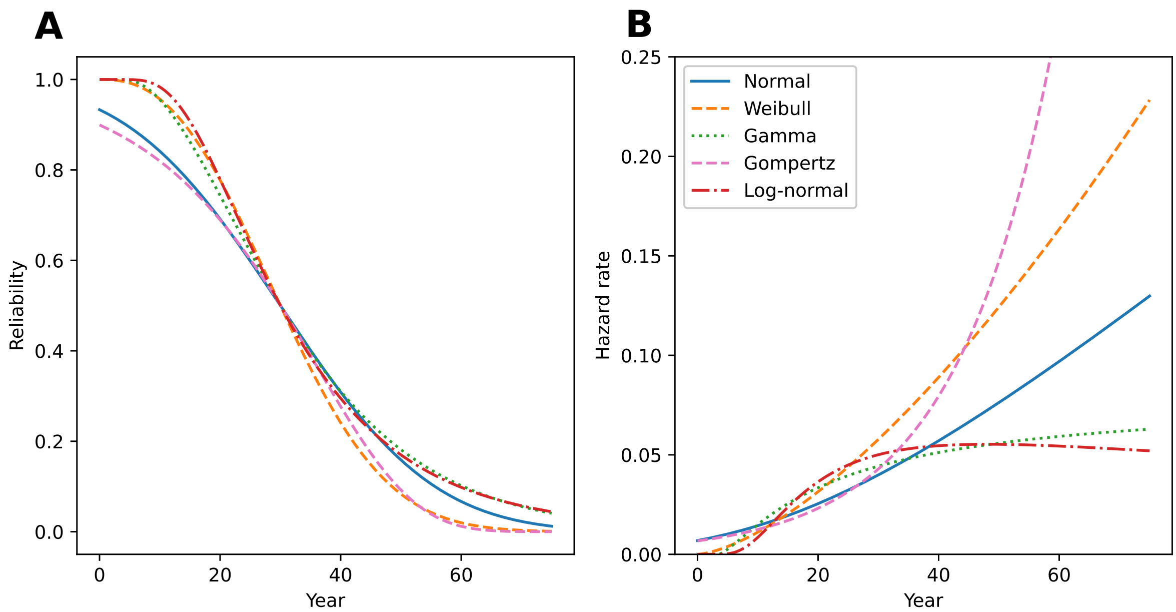

Figure 1.4: Survival curves (a) and hazard rate (b) of multiple distributions. All displayed distributions have the same median value (50 % in $t = 30$) and the same standard deviation ($\sigma = 20$). The figure is inspired by Miatto et al. (2017).

It is important to notice that following descriptions and observations of the distributions are not all generalizable since shape and location may vary based on the parameters defining the distribution. The displayed distributions in Figure 1.4 can be categorized in right-skewed distributions (Weibull, Lod-normal, and Gamma), left-skewed distributions (Gompertz), and the normal distributions. The individual properties of the distributions need to be considered when a distribution is selected to model a stock decay. Looking at the displayed right skewed distributions it is apparent that the first value of the survival curve is 1, meaning that the whole basic population survived till that point. This is not the case for the displayed normal distribution since its value in the survival curve is below 1. Hence, by using the normal distribution with these settings to model a survival curve it must be assume that the stock depletion starts right at the moment of material input. Regarding buildings this implies demolition of some buildings right after construction (Miatto et al., 2017) and for consumer electronics it assumes that part of the stock is discarded within a year. Also the Gompertz distribution has specific implications since it is normally used to model lifetimes of living beings. Because living beings cannot exceed a certain age (humans currently day latest around 120 years of age ("List of the verified oldest people", 2022)) the hazard function of the Gompertz distribution (see Figure 1.4 B) grows exponentially once stabilized (Miatto et al., 2017). If the Gompertz function would be applied to to buildings it had to be assumed that no building exceeds a certain maximum lifetime.

Using this knowledge, one can pick a distribution based on assumptions. Those could be the following for buildings:

- Recently build infrastructure is unlikely to get demolished in the year of construction.
- There will be a peak at in stock depletion depending on external factors as location and typology.
- Buildings surviving this peak are probably deemed to be worth preserving resulting in a lifetime far beyond average.

On this basis, it can be assumed that the log-normal distribution may be the best to model the stock decay of buildings. Miatto et al. (2017) test this assumption by fitting multiple distributions on historical data of three locations. It turned out that right skewed distributions describe stock dynamics indeed well. However, only when the underlying assumptions can be preserved throughout the lifetime. The example of the city of Salford in the United Kingdom proves the point. During the 20th century Salford went through an economic boom, followed by an economic crisis which led to the construction of inferior houses. A large share of those were demolished within a short period. As a consequence of this dynamic, the Gompertz distribution (left skewed) is most suitable in this case.

Since survival curves in dynamic MFAs are used to model an uncertain future, it may not be possible to foresee events as described. Therefore, the selection of a distribution can only be based on the knowledge available in the very moment of modelling. For those reasons assumptions on distribution shapes can turn out wrong when modelling results are compared with reality (Ianchenko et al., 2020). Furthermore, data on survival curves can rarely be applied to another local or temporal context since the systems scope really matters (Ianchenko et al., 2020; Yu et al., 2020).

In conclusion, it is possible to make an educated selection regarding the distribution of a survival. However, it is possible that made assumptions will turn out wrong due to unforeseen events. Furthermore, as demonstrated in Section 1.1.3 it is often difficult to obtain valid data on lifetimes. Therefore, lifetimes and their distribution pose a major source of uncertainty in dynamic MFA modelling.

1.2. Research gap and research questions

Section 1.1.3 shows that modelling reuse is complex. The data is obtained through conducting surveys and interviews, and the derived survival curves are objected to uncertainties. Presumably because of the high effort required, detailed reuse modeling as suggested by Thiébaud et al. (2017) has not been integrated into any MaTrace model yet. Therefore, the first objective of this research is to integrate Thiébaud et al. (2017) reuse model into an existing MaTrace model. This objective dictates the main research question:

How to introduce reuse into a MaTrace model and how to evaluate it?

The chosen model is the MaTrace model on cobalt in the European Union of Godoy León et al. (2020) (for more information see Section 1.3 and Section 2.1). The model created out of Thiébaud et al. (2017) reuse model and Godoy León et al. (2020) MaTrace model will be referred to as the **Reuse-MaTrace model** in the following. Once the Reuse-MaTrace model is created, the first research objective is to understand if this integration has a substantial impact. This leads to the first sub-research question:

To what extent is the outcome of the MaTrace model as described by Godoy León et al. (2020) altered, when the reuse of consumer electronics is modelled following the approach of Thiébaud et al.

(2017)?

The combination of those two models is possible since Glöser-Chahoud et al. (2019) applied Thiébaud et al. (2017) reuse model on electronics in Europe in a similar temporal scope. This endeavour requires only a minimal data gathering effort. The data present is, however, subject to uncertainty as described in Section 1.1.4. Furthermore, the lifetime of each product is represented by a survival curve and as described in Section 1.1.5 it is hard to pick the correct distribution and to find the right parameter settings. Also the data used in the MaTrace model of Godoy León et al. (2020) is not fully certain and the data quality varies depending on the parameter as they show in their previous publication (Godoy León & Dewulf, 2020). These circumstances lead to the second sub-research question:

Which input parameters introduce the most uncertainty into the Reuse-MaTrace model and what insights can be derived from analysing uncertainties?

The following section gives an introduction to cobalt as chosen material to conduct this research.

1.3. A case study on cobalt

The chosen material for this research is cobalt. Cobalt is a core material of rechargeable batteries due to its unique properties. Two current trends drive the demand for rechargeable batteries. On the one hand, the need to transition from fossil fuels to renewable energies kicked off. Electrification in the automotive industry makes electric vehicles (EV) the current, and future, main driver for demand of cobalt (Sun et al., 2019). The energy transition will require energy storage capacities (e.g., home battery storage) which will also drive the demand in the future. This leads to cobalt being considered as an energy transition metal (ETM) (Rachidi et al., 2021). On the other hand, the ongoing digitalization of industry and private life also considering trends as internet of things (IOT) and 5G technology will drive the demand for portable batteries (Desai, 2020). Certainly, this will increase the demand in the foreseeable future.

Although, the above listed driver suggest an increase in demand advancements in battery development may counteract in the future. A large electronic vehicle producer already uses cobalt-free batteries (McFarland, n.d.) while researchers use scenarios in which the cobalt demand declines in 2030 due to changes in battery technology (Tang et al., 2021). Hence, the future cobalt demand is uncertain.

The above outlined development concerns the main source of virgin cobalt. More than two thirds of the global cobalt supply is sourced in the Democratic Republic of Congo (DRC) (Farchy & Warren, 2018) where insecure mining conditions and reoccurring human rights violations such as child labor occur (Sovacool, 2019). Due to its relevance for the energy transition and the problematic origin of the virgin material I consider cobalt a material worth studying.

Looking at the publications treating cobalt using dynamic MFA (search on Scopus using the terms "cobalt AND dynamic "material flow analysis"" and "cobalt AND dynamic MFA") it is striking that the overwhelming majority has been published during the last three years. Accordingly, the publications of Pehlken et al. (2017), Bobba et al. (2019), Kamran et al. (2021), and Tang et al. (2021) entail prospective dynamic MFAs treating CRMs in EV batteries which cover cobalt as well. The regional and temporal scope vary. Furthermore, those publications also treat circular strategies as reuse, recycling and shared ownership to varying extends. In contrast Kastanaki and Giannis (2022) focuses on the future global CRM demand caused by smartphones. More broadly, Dunn et al. (2021) investigates the global CRM demand caused by batteries and considers circular scenarios.

Additionally, three publications were found conducting retrospective dynamic MFAs. Liu et al. (2021) investigates lithium and cobalt flows in China while Wang and Ge (2020) solely focus on cobalt flows in China. Godoy León et al. (2022) quantify long term cobalt stocks and flows in the European Union.

The only MaTrace model found which treats cobalt is the one of Godoy León et al. (2020) which traces the cobalt inflow of 2015 within the European Union.

On the basis of this review it can be concluded that the energy transition, especially regarding vehicles motivated a large share of the presented studies. As a consequence only few publications solely treat cobalt. Furthermore, many studies investigate the impact of circular strategies as it will be done in this research. The novelty of the Reuse-MaTrace model is the integration of an elaborate reuse model into a MaTrace model. The creation of the model and whether the integration of reuse has a meaningful impact will be discussed in the following chapters.

2
Methodology

This chapter describes the actions taken in order to answer the research questions. The modelling approach will be described first. The MaTrace model was extended to consider the potential reuse of consumer goods (see Section 2.1). Because the model is far from trivial, the actual implementation of the model is explained (see Section 2.2). Apart from the modelling itself, the impact of the suggested changes and the model behaviour are relevant. An impact analysis to gain knowledge on this will be performed (see Section 2.3). The MaTrace model itself requires a lot of data and the model input will be inflated due to the proposed extension (also see Section 2.4.1 where the inputs are mapped out). For this reason, Monte Carlo simulations are conducted to gain knowledge about the relevance of all inputs (see Section 2.4).

2.1. Modelling approach

The foundation of the research project is a MaTrace model which considers reuse as described in Section 1.1.3. Since such a model does not exist yet, two models needed to be combined. I deemed the MaTrace model developed by Godoy León et al. (2020) to be suitable. As displayed in Figure 2.1, the model follows the generic MaTrace approach by incorporating a use, EOL and a production phase (also see Section 1.2). Exports and different losses are considered. Besides the pretreatment and recycling losses, which occur due to process efficiencies, the model considers downcycling and non-selective collection. Here downcycling refers to material which ends up in low tech products. In the context of cobalt this mainly applies to alloys containing cobalt which are then downcycled into stainless steel. In this case the material is dissipated into the technosphere (Godoy León et al., 2020) from where it is in general not recoverable (Godoy León et al., 2020). Non-selective collection refers to the misplacement of EOL products into the wrong waste bin (Godoy León & Dewulf, 2020). In contrast to the original MaTrace model, this model considers hibernating stocks (Godoy León et al., 2020).

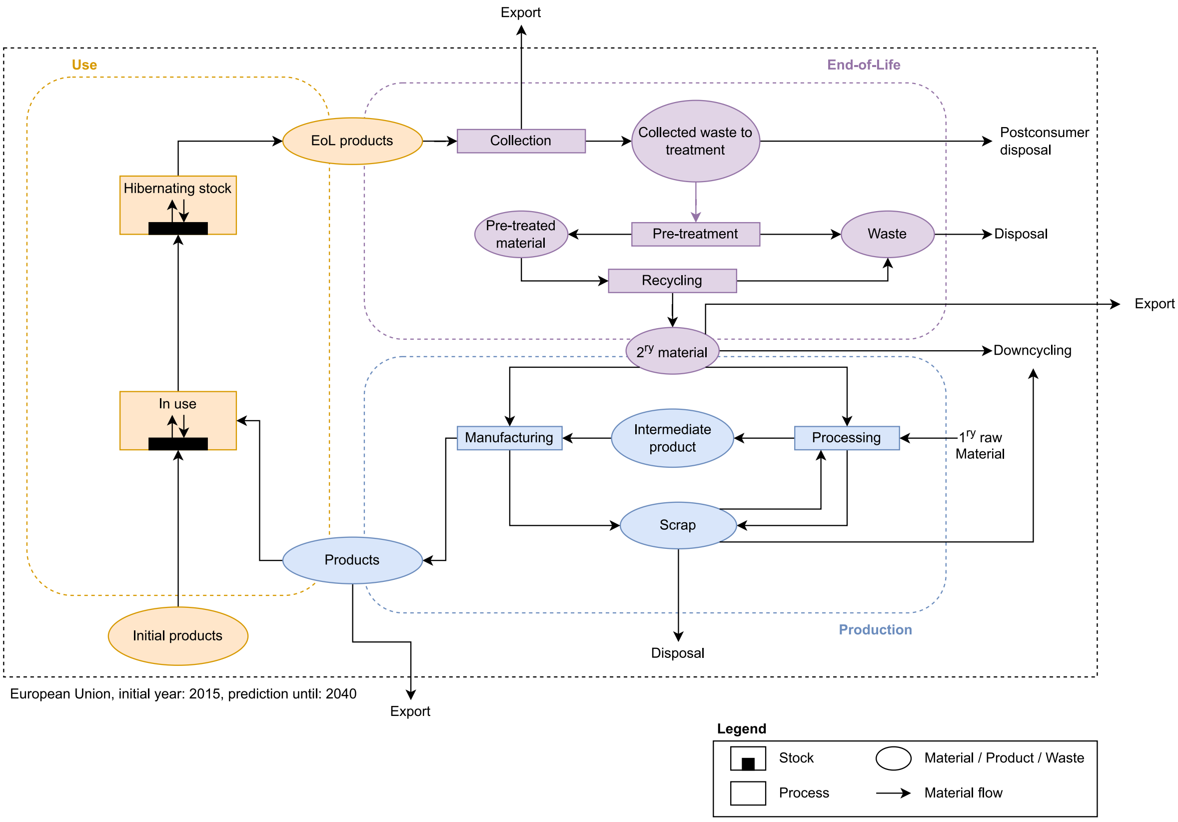

Figure 2.1: MaTrace model system diagram by Godoy León et al. (2020)

The model is suitable due to the distribution of initial inflow as well as its consideration of cobalt, which makes it highly relevant. It considers eleven product categories: Portable batteries, mobility batteries, three types of catalysts, dissipative uses, hard metals, magnets, other metallic uses, and superalloys. 41.2 % of the whole in-flowing cobalt is allocated to portable batteries (Godoy León et al., 2020). The category portable batteries covers rechargeable batteries in consumer electronics such as laptops, cell phones, and cameras (Godoy León & Dewulf, 2020). Chapter 1 describes that the total demand for portable batteries will increase while the demand relative to the total cobalt demand may decrease. It is predicted that 30% of the cobalt used in batteries today will be used in portable batteries in 2025 (Desai, 2020).

In order to model the reuse of this portable batteries category I will extend the MaTrace model by Godoy León et al. (2020) with the reuse model of Thiébaud et al. (2017) (see Figure 2.2).

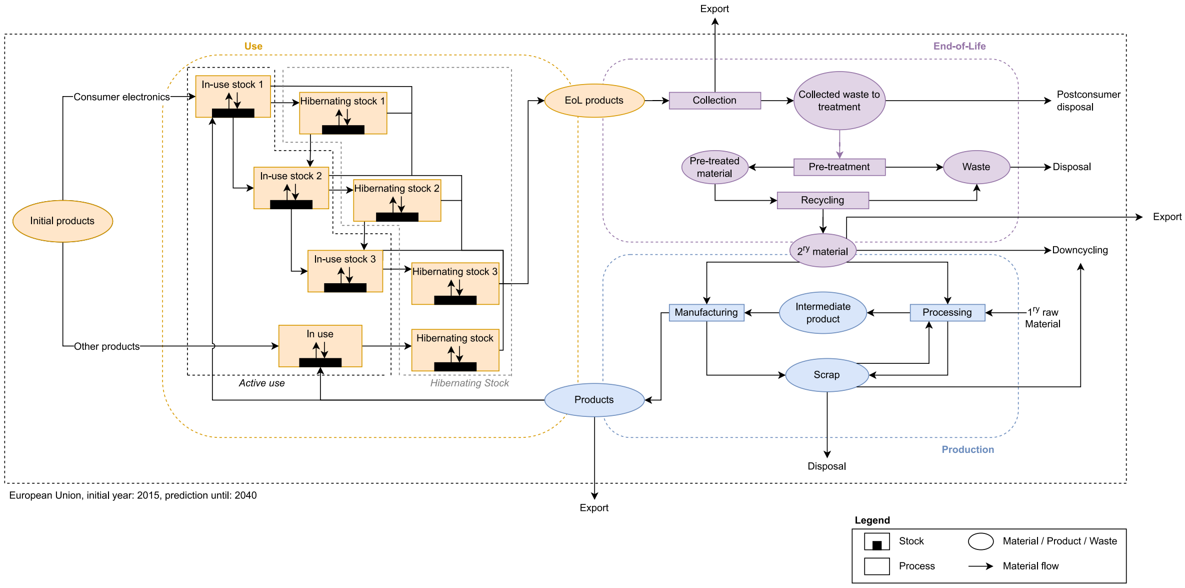

Figure 2.2: Reuse-MaTrace model system diagram

Besides the data as used by Godoy León et al. (2020) in the MaTrace model, the extended reuse part relies on data as presented by Glöser-Chahoud et al. (2019) who applied the reuse model by Thiébaud et al. (2017) on Europe. This data already shows strong tendencies towards reuse. According to Glöser-Chahoud et al. (2019) 60% of smart phones in Europe are reused, and 14 % have more than two owners. In addition to this already high reuse rate it can be assumed that the second hand market will grow in the future. Also because of the growing popularity of second hand e-commerce platforms Glöser-Chahoud et al. (2019). Figure 1.3 shows that the original reuse model also considers the fate of the disposed products. In the combined model, the outflow will be summed up and passed back to the MaTrace model which handles the fate of the disposed products.

The following section explains the functionalities of the combined model.

2.2. Model implementation

Figure 2.2 displays, the start of model, the use phase has two inputs; the initial products and products produced from secondary materials in the production phase. Thus, there is only one inflow from outside the system boundaries. In order to determine the inputs to the use phase of the second year, the whole model has to be executed for the initial year first. The material leaving the use phase has to pass through the end-of-life phase. Retrieved secondary material will be used in the production phase to produce new products. A share of those products become the inflow into the use phase of the second year. Therefore, the model has to be run iteratively.

In the first iteration, the initial inputs enter the system and get split up. Portable batteries enter the cascaded reuse model, all other categories are treated as in the MaTrace model: they enter a use stage and one hibernating stage afterwards. Within the reuse model the inflow is split into seven products with individual data on service lifetime, hibernating time (represented by survival curves), and reuse (represented by transfer coefficients) (Also see Chapter 3).

All stocks, in-use and hibernating, are represented by one cohort matrix per product (in reuse model) or per product category (as in MaTrace model by Godoy León et al. (2020)). A cohort matrix represents the net-inflow, the stock itself, and the depletion of a stock. It is created by the inflow and the survival curve.

	0	1	2	3	4	5	6	7
0	0	0	0	0	0	0	0	0
1	0	0.005779	0	0	0	0	0	0
2	0	0.004155	0.009849	0	0	0	0	0
3	0	0.002126	0.007081	0	0	0	0	0
4	0	0.000853	0.003623	0	0	0	0	0
5	0	0.000279	0.001454	0	0	0	0	0
6	0	7.59E-05	0.000475	0	0	0	0	0
7	0	1.75E-05	0.000129	0	0	0	0	0

Table 2.1: Cohort matrix representing the 2nd in-use stock of smart phones until the third iteration

Table 2.1 displays the cohort matrix of the second in-use stock (first reuse stock) of smartphones after the third iteration. The diagonal of the matrix holds the stock addition in each year, which is not necessarily equal to the inflow, since inflow may already partly decay during the first year. This depends on the distribution used for the survival curve (also see Section 1.1.5). The inflow multiplied with the survival curve defines one column. Hence, one column provides the knowledge, how much was added to a stock in one year (entry on the diagonal) and how much of this addition is in stock in the following years. Due to this circumstance, one finds the total material in stock of a year by summing a row (derived from B. Müller (2006)). Because of the iterative nature of the model, the matrix is not fully filled after two iterations. Furthermore, since the stock outflow is put into the MaTrace model, it might be that a former outflow flows back into the stock at some point. Table 2.2 shows the cohort matrix of the second in-use stock of smart phones when the model is run for eight iterations.

	0	1	2	3	4	5	6	7
0	0	0	0	0	0	0	0	0
1	0	0.005779	0	0	0	0	0	0
2	0	0.004155	0.009849	0	0	0	0	0
3	0	0.002126	0.007081	0.009332	0	0	0	0
4	0	0.000853	0.003623	0.00671	0.007348	0	0	0
5	0	0.000279	0.001454	0.003433	0.005283	0.005278	0	0
6	0	7.59E-05	0.000475	0.001378	0.002703	0.003795	0.003532	0
7	0	1.75E-05	0.000129	0.00045	0.001085	0.001942	0.00254	0.002184

Table 2.2: Cohort matrix representing the 2nd in-use stock of smart phones until the eighth iteration

The first column of the matrix only holds zeros. This suggests that there is no inflow to the second use-stock in the first year. Only in the second iteration the first in-use stock starts to deplete and part of the phones leaving the first in-use stock enter the second.

Within the reuse model in the use phase transfer coefficients define which share of a stock outflow goes to either the next use-stock, the hibernating stock, or to disposal. Since the MaTrace model incorporates the waste treatment process including losses and exports, the reuse model considers only one disposal way resulting in the EOL products. In order to suit the MaTrace model, the individual product outflows of the reuse model are summed up into the category *portable batteries* again.

The clusters End-of-Life and Production are equivalent to the MaTrace model by Godoy León et al. (2020). Both clusters are defined by transfer coefficients and allocation matrices. Furthermore, a infinite geometrical series emerges due to the close loop in the production cluster. This series is solved analytically (see Section 1.1.2).

2.3. Impact analysis

The impact analysis serves the purpose to investigate how the output of the MaTrace model is altered due to the modification. I chose the total in-use stock as the measure of comparison since this model output is closely related to resource efficiency (see Section 1.1.2). The impact analysis consist of the following two steps: Comparison to the MaTrace model by Godoy León et al. (2020) and the impact of reuse.

2.3.1. Comparison to the MaTrace model created by Godoy León et al. (2020)

Firstly, it will be investigated how the in-use stock changes once the reuse model is added. In a second step the impact of the usage of an altered data set (see Section 3) will be examined. Based on this analysis it will be possible to answer, whether the consideration or reuse is of relevance at all regarding this specific case study.

2.3.2. Impact of reuse

Secondly, the impact of the consideration of reuse is evaluated in greater detail. To do so, the part of the model considering reuse (see marked area Figure 2.3 A) is altered. In order to create a baseline, the reuse model is reduced to showcase single use only (see Figure 2.3 B). Then the model is run with two use stages (see Figure 2.3 C) and then with three (see Figure 2.3 D).

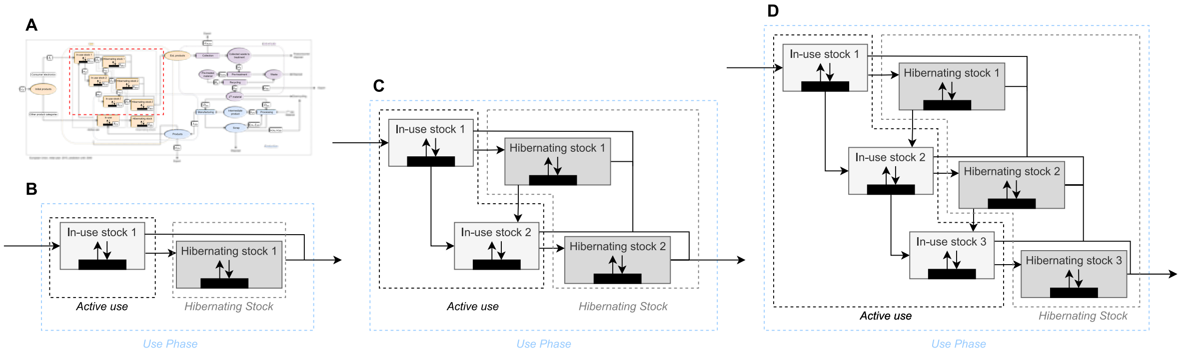

Figure 2.3: Scenarios for the reuse impact analysis; (b) considering single use, (c) considering one reuse phase, and (d) considering the whole reuse model. The red dotted line in (a) marks the location of the use phase in the whole system.

The results of this analysis will allow to draw conclusions on the impact of the consideration of reuse on the in-use stock.

2.4. Monte Carlo simulations

Monte Carlo methods are used in different scientific fields for various purposes (Dimov, 2008) and are formally defined as: "methods of approximation of the solution to problems of computational mathematics, by using random processes for each such problem, with the parameters of the process equal to the solution of the problem." (Dimov, 2008, p.1)

In summary, the inputs of a model which have an effect on the solution (or model output) are varied in a random fashion. When applied on MFA models, selected or all inputs are defined by a probability distribution. Random inputs are generated on the basis of those distributions which are then fed into the model. This process is repeated multiple times. As a result, one obtains probability distributions of the output data (Sonnemann et al., 2003). It is important to understand, that inputs are not varied arbitrarily randomly but that the inputs are generated on the basis of the assigned probability distribution). This also entails to set limits of the number generator to a plausible range. Furthermore, not all values have the same probability to be generated.

Besides the more obvious result of the probability distributions of outputs, one can derive further conclusions by analyzing the results. In the context of MFA, Monte Carlo simulations are used to analyze the uncertainty and sensitivity of models (Fishman et al., 2018). In this case that is also the purpose. The presented combined model is unique and unproven. Although, the data was mainly collected from previous peer reviewed publications, the authors of these publications recognize the weaknesses of the data quality themselves. Godoy León and Dewulf (2020) evaluated the data quality of each input used in the MaTrace model by Godoy León et al. (2020) while Thiébaud et al. (2017) stressed that the data for the reuse model has to be obtained by interviews and surveys. Hence, knowing which inputs have the largest impact on relevant outputs is important information in case practitioners consider to use the model in the future. This way, users can know which inputs require a high certainty (i.e. data quality) and which inputs require less attention.

Even though, the method appears to be established in MFA modelling, approaches on how to assign probability distributions to inputs vary among publications. It seems common to assign distributions on the basis of the known uncertainty of the inputs (Cai et al., 2022; Cao et al., 2018; Fishman et al., 2018; Glöser et al., 2013; Gottschalk et al., 2010; Montangero & Belevi, 2008; Thiébaud et al., 2018). But the derived distributions vary immensely. Fishman et al. (2018) used exclusively normal distributions, while Thiébaud et al. (2018) use triangular and normal distributions for inputs with higher certainty. Montangero and Belevi (2008) derives most input distributions including parameters from existing literature, and Gottschalk et al. (2010) uses log-normal, triangular or uniform distributions depending on input characteristics.

On the one hand this poses the challenge to execute Monte Carlo simulations without clear guidelines. On the other hand, it allows to develop a framework according to the needs of the model and researcher. In order to develop this framework, the following section maps out all inputs of the model. On the basis of this knowledge a framework to assign distributions will be developed.

2.4.1. Model input mapping

The data inputs to the model need to be mapped to create an overview. Furthermore, the total number of inputs is calculated in this section.

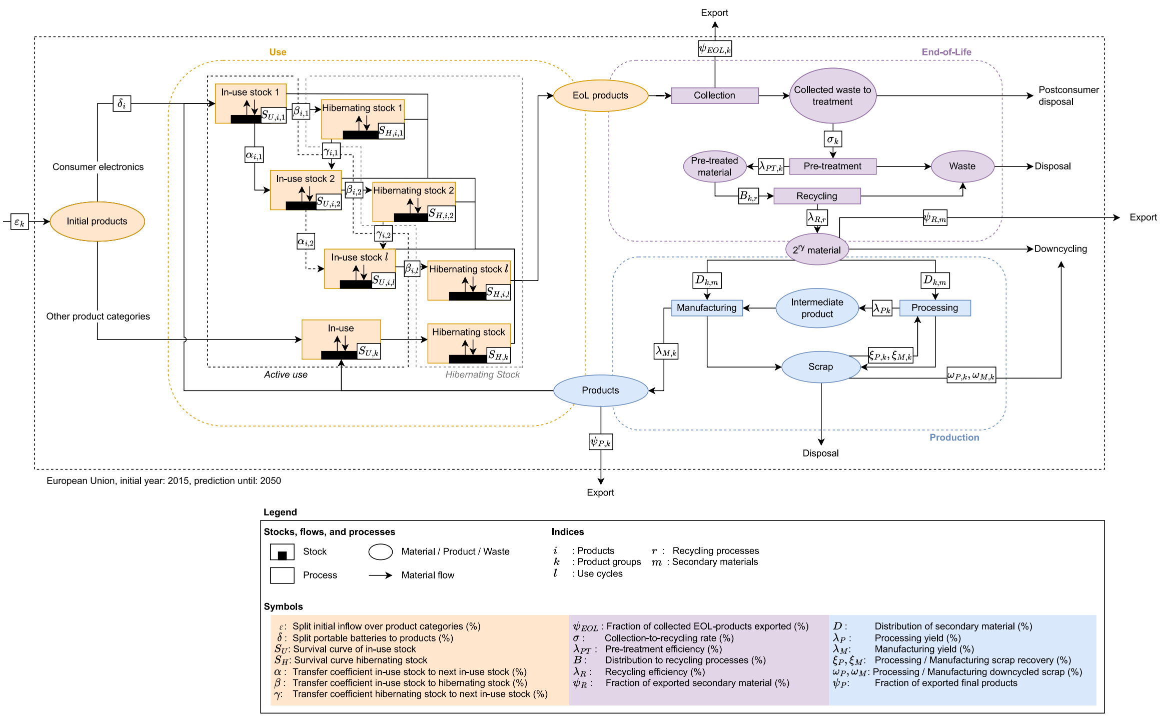

Figure 2.4: Reuse-MaTrace model and required data (adopted from Godoy León et al. (2020))

Figure 2.4 displays the system and data required to run the model, which are represented by boxes holding mathematical symbols. Each symbol has one or more indices (small letters) indicating whether this data is required for each product (index i, consumer electronics as e.g., laptops), product group (index k, e.g., hard metals), use cycle (index l, referring to use- and reuse- cycles not recycling), recycling process (index r, recycling processes as present in MaTrace model), or secondary materials (index m, material created by recycling processes). If multiple indices are given, the data is required for every combination (e.g. $S_{U,i,l}$ represents the in-use survival curve and it is required for every product in every use-cycle). I calculated the number of individual inputs on the basis of Figure 2.4. Therefore, a norm must be defined which gives the number of elements in a vector or matrix of the dimensions $\mathbb{R}^{p \times q}$:

$$||A||_R = \sum_{j=1}^{p} \sum_{h=1}^{q} 1 \tag{2.1}$$

Considering the seven products (index i), 11 product groups (index k), three use cycles (index l), two recycling processes (index r), and two secondary materials (index m) one finds the following table by applying the $||A||_R$ norm:

Vector or Matrix	Dimension	Number of elements
ε	$k \times 1$	11
δ	$i \times 1$	7
α	$i \times l - 1$	14
β	$i \times l$	21
γ	$i \times l - 1$	14
ψ_{EOL}	$k \times 1$	11
σ	$k \times 1$	11
λ_{PT}	$k \times 1$	11
B	$k \times r$	22
λ_R	$r \times 1$	2
ψ_R	$m \times 1$	2
D	$k \times m$	22
λ_P	$k \times 1$	11
λ_M	$k \times 1$	11
ξ_P	$k \times 1$	11
ξ_M	$k \times 1$	11
ω_P	$k \times 1$	11
ω_M	$k \times 1$	11
ψ_P	$k \times 1$	11

Table 2.3: Dimensions and number of input parameters

The sum of all elements is 225, while the part of the model which treats the reuse of consumer electronics requires 56 inputs. However, Table 2.3 does not consider the number of the required survival curves which is displayed in the following table:

Survival curve	Number of survival curves
S_U	$i \cdot l + k - 1 = 31$
S_H	$i \cdot l + k - 1 = 31$

Table 2.4: Number of required survival curves

In the combined model, all survival curves are defined by Weibull distributions, described by two parameters. Thus, the original model has $62 \cdot 2 + 225 = 347$ input parameters. If the distribution describing the survival curves is changed during the course of the experiments, this number can vary.

Hence, the part of the model which treats the reuse of consumer electronics requires 56 inputs and 42 survival curves (82 additional inputs).

2.4.2. Framework

The number of input parameters is too large to define a specific distribution for each, which means that an alternative, feasible approach needs to be applied. This approach consists of two steps. Firstly, each input is going to receive a score mainly based on uncertainty and where known by sensitivity. Secondly, these scores will be used to assign a distribution to each input.

Input scoring

Scoring is a commonly used practise in the field of IE to compare things as the impacts of multiple environmental interventions. Often multiple categories are scored on the basis of qualitative or quantitative information and one main score is aggregated (Duc et al., 2022; van Berkel et al., 1997). The main drawback is the low repeatability of the score assignment (Powell et al., 1997). Therefore, I explain how scores were assigned in the following.

The model contains five different input data types: the initial inflow, transfer coefficients, efficiencies, the Weibull scale, and the Weibull shape. The first four types can receive an uncertainty score from 0 to 5. Here, 0 represents absolute certainty and 5 stands for very high uncertainty. An example for an absolute certain input is the recycling efficiency of dissipative uses. In MaTrace models dissipative uses are the use of material in e.g., medicine or pesticides or regarding cobalt, the use of the material as pigment. So, the material cannot be recovered by definition. Therefore, the recycling efficiency for cobalt recovery from dissipative uses is 0 with absolute certainty. The score of 5 was assigned for inputs which are based on my own assumptions.

The Weibull shape parameter β can only receive scores from 0 to 2. The reason for this is its known sensitivity. The shape of the Weibull distribution can change severely when the parameter varies. Figure 2.5 A displays the survival curves of smartphones in the first service phase considering multiple shape parameters. When $\beta > 1$ as for the original shape ($\beta = 1.7$) the failure rate increases over time (see Figure 2.5). As a result, few smartphones fail during the fist two years and most of them drop out of service between the second and the third year. This behaviour changes for $\beta \approx 1$ which leads to a more constant failure rate. For $\beta < 1$ the failure rate is high at the beginning and decreases over time. As it can be seen in Figure 2.5, this leads to an early failure behaviour. Less than half of the smart phones survive the first two years (Kızılersü et al., 2018). For this known sensitivity of the Weibull shape, the uncertainty scores are limited to the mentioned range.

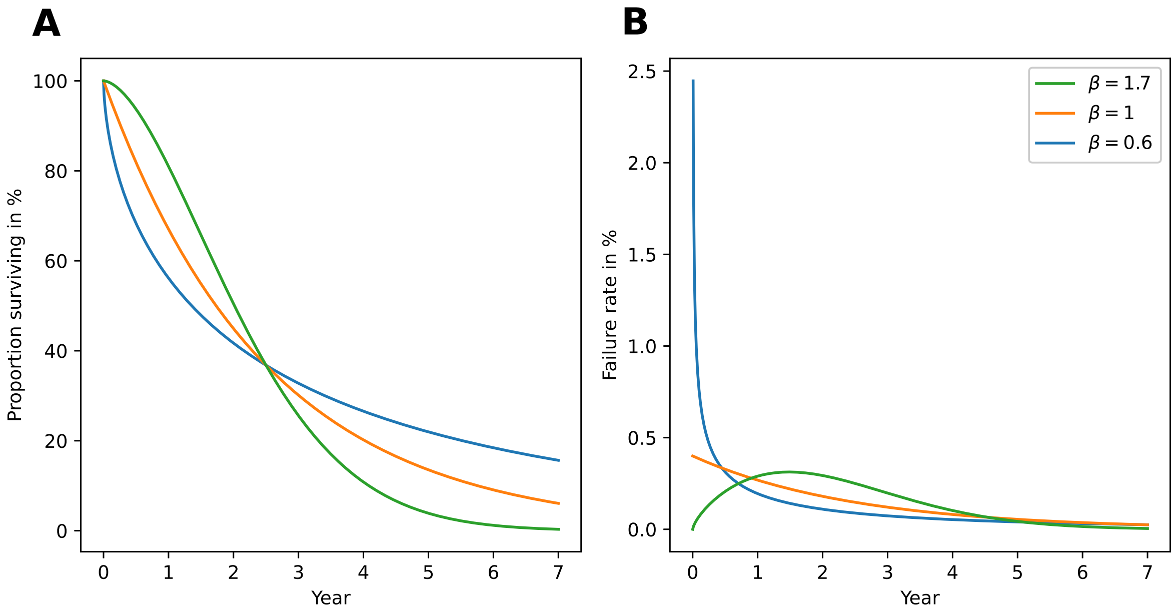

Figure 2.5: Survival curve (a) and probability density function/failure rate (b) of Weibull distribution for multiple shape parameter β

The inputs which come from the MaTrace model by Godoy León et al. (2020) are scored on the basis of a previous publication of the same authors. Godoy León and Dewulf (2020) developed a framework to asses the quality of CRM related data. This framework was applied to the MaTrace model which is used in this thesis. Hence, the data quality of each input to the MaTrace model was scored from "Very high data quality" over "High data quality", "Low data quality", and "Very low data quality" to "No data reported" (Godoy León & Dewulf, 2020, Table 3). This data quality stands in direct relation to data uncertainty. High quality data is more reliable and therefore more certain. The data quality evaluation of Godoy León and Dewulf (2020) is translated as follows:

- Uncertainty score 1: "Very high data quality"
- Uncertainty score 2: "High data quality"
- Uncertainty score 3: "Low data quality"
- Uncertainty score 4: "No data reported"

The category "Very low data quality" does not refer to an uncertainty score, since this category was not assigned to any input. Furthermore, the category "No data reported" was matched with the uncertainty score 4, since Godoy León et al. (2020) filled in missing data based on their research, assumptions, and expertise. Because I assume that the validity of their data assumptions is more valid than the data which bases on my own assumption, this kind of data did not receive the lowest score.

The uncertainty of the data which originates from Glöser-Chahoud et al. (2019) application of Thiébaud et al. (2017) reuse model is scored by my own judgement. Regarding the first use and storage phase it is assumed that the survival curves defined by Glöser-Chahoud et al. (2019) have a high certainty as they are based on multiple empirical studies. Accordingly, the shapes receive a uncertainty score of 1 and the scales receive an uncertainty score of 2. Since the survival curves of the products e-bikes, power tools, and others base on own research, they are scored lower. Weibull scales received a score of 4 and Weibull shapes a score of 2. The transfer coefficients as suggested by Glöser-Chahoud et al. (2019) are derived from previous research (survey and interview studies) thus they are assumed to be less certain and receive an uncertainty score of 3. The transfer coefficients for e-bikes, power-tools, and other products are scored with 4 since they are based on literature and derived assumptions (see Chapter 3).

For the second re-use and storage stage I assumed that the data is less certain than the data of the first stage. The data of the reuse model largely depends on surveys and interviews (Thiébaud et al., 2017). I assumed that the information gathered becomes vague in the second stage since part of the information provided is less certain. It is for example less likely that owners of second hand articles know the exact purchase date because they may not have a receipt. Furthermore, they might not be aware of all previous owners and may mistake a third hand product for a second hand product. In order to account for those kind of added uncertainty, I lowered all all uncertainty scores by one.

Regarding the third re-use and storage stage I assumed that the data is not certain at all. The aforementioned uncertainties are present as well. Furthermore, owning a third hand product is less likely than owning a second hand product. Therefore, the pool of possible survey and interview participants must have been smaller. All inputs on this stage are thus rated with the highest uncertainty possible, which is 2 for Weibull shapes and 5 for all other parameters.

Appendix B shows assigned uncertainty scores of all inputs.

Distributions

As explained above, the uncertainty scores are used to assign distributions to the inputs. How this is done will be explained in the following. The fundamental idea is to assign broader distributions to uncertain inputs and narrow distributions to inputs with a high certainty. This results in the following pairing for this Monte Carlo simulation:

- Uncertainty score 0: The input value is not changed at all
- Uncertainty score 1: The input value is altered by a normal distribution
- Uncertainty score 2: The input value is altered by a broader normal distribution
- Uncertainty score 3: The input value is altered by a triangular distribution
- Uncertainty score 4: The input value is altered by a broader triangular distribution
- Uncertainty score 5: The input is very uncertain and therefore altered by a uniform distribution (Gottschalk et al., 2010)

The specific parameters of the distribution depend on the type of input data. The initial inflow, transfer coefficients, and efficiencies can take values from 0 to 1 while the Weibull scale and shape can take theoretically arbitrary values larger than 0. Therefore, those groups of input are treated differently.

Regarding the Weibull scale and shape, the distribution does not alter the input value directly but the distributions generate a multiplier for the input. The multiplier can take values from 0.5 to 1.5. So, the input value can be 50% larger or smaller than the initial value. The distributions for uncertainty scores 3 to 5 are limited to this range. If a normal distribution for the uncertainty scores 1 and 2 generates a value out of this range, a new value will be generated until it is within this range. Figure 2.6 A displays the distributions for this case:

- Distribution for uncertainty score 1: Normal distribution with $\mu = 1$ and $\sigma = 0.05$
- Distribution for uncertainty score 2: Normal distribution with $\mu = 1$ and $\sigma = 0.1$
- Distribution for uncertainty score 3: Triangular distribution limited from 0.6 to 1.4 with the peak at 1
- Distribution for uncertainty score 4: Triangular distribution limited from 0.5 to 1.5 with the peak at 1
- Distribution for uncertainty score 5: Uniform distribution limited from 0.5 to 1.5

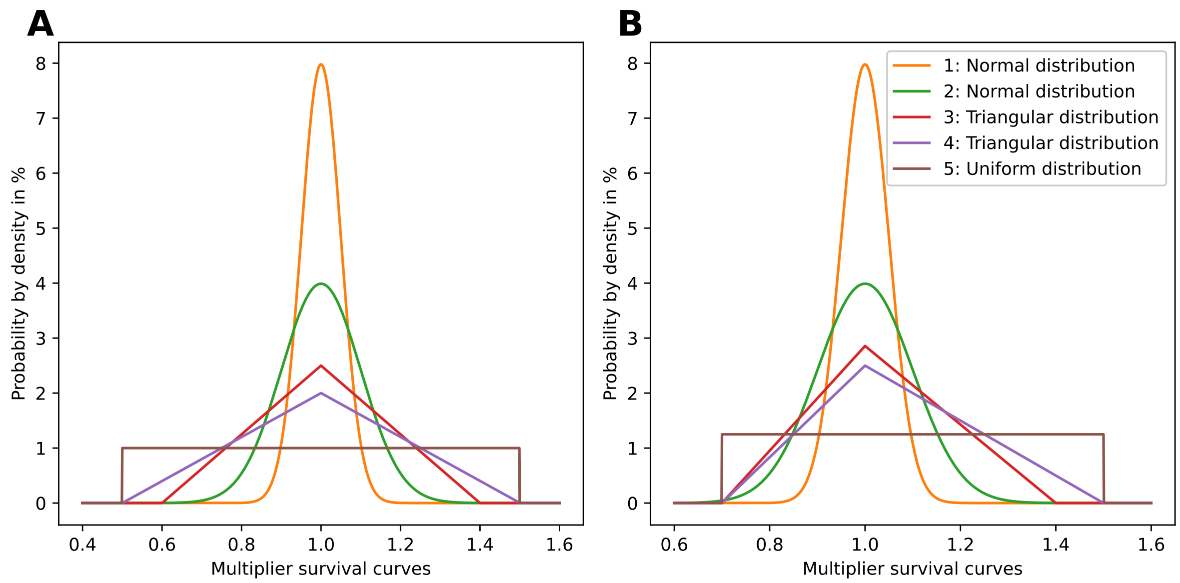

Figure 2.6: Distributions of survival curve multiplier for Monte Carlo simulations. (a) shows the distribution without limitations. (b) shows the distributions when the smallest possible multiplier is limited to 0.7.

As explained above, the Weibull scale β changes the shape of the survival curve severely when it changes from $\beta > 1$ to $\beta < 1$. Therefore, it was decided that Weibull scales which are initially larger than 1 cannot take values smaller than 1. To ensure this, the smallest possible multiplier for which $\beta \leq 1$ is calculated and used as the lower limit for all distributions (see Figure 2.6 B, here the smallest possible multiplier is 0.7). The normal distributions generate values below this threshold, new values are generated until all values are within the allowed range.

The same applies for the Weibull shapes: A shape below 1 would suggest that most of the stock depletes during the first year which is, looking at the data, for most products and cases an unreasonable assumption. Furthermore, the Weibull survival curve always has a value of 1 for the input year. Hence it cannot project stock depletion in the first year. Furthermore, transfer coefficients define in most cases the inflow to the stocks. Therefore, there is no need for the survival curve to represent inflows that immediately exit.

In contrast to the Weibull parameters the distributions for initial inflow, transfer coefficients, and efficiencies take the actual input value as a mean for the normal distributions and as peak for the triangular distributions. The general settings are as follows:

- Distribution for uncertainty score 1: Skewed or folded normal distribution with $\mu = 1$ and $\sigma = 0.05$
- Distribution for uncertainty score 2: Skewed or folded normal distribution with $\mu = 1$ and $\sigma = 0.1$
- Distribution for uncertainty score 3: Triangular distribution limited from 0.6 to 1.4 with the peak at 1
- Distribution for uncertainty score 4: Triangular distribution limited from 0.5 to 1.5 with the peak at 1
- Distribution for uncertainty score 5: Uniform distribution limited from 0.5 to 1.5

Figure 2.7 A displays the distributions when the input value is 0.5, the distributions for other values change. Figure 2.7 B shows the distributions for an input value of 0.2. It shows that the distribution for uncertainty score 1 changes to a right skewed normal distribution. The reasoning behind this implementation is that it might be interesting for small values to test how the model behaves for larger values rather even smaller inputs.

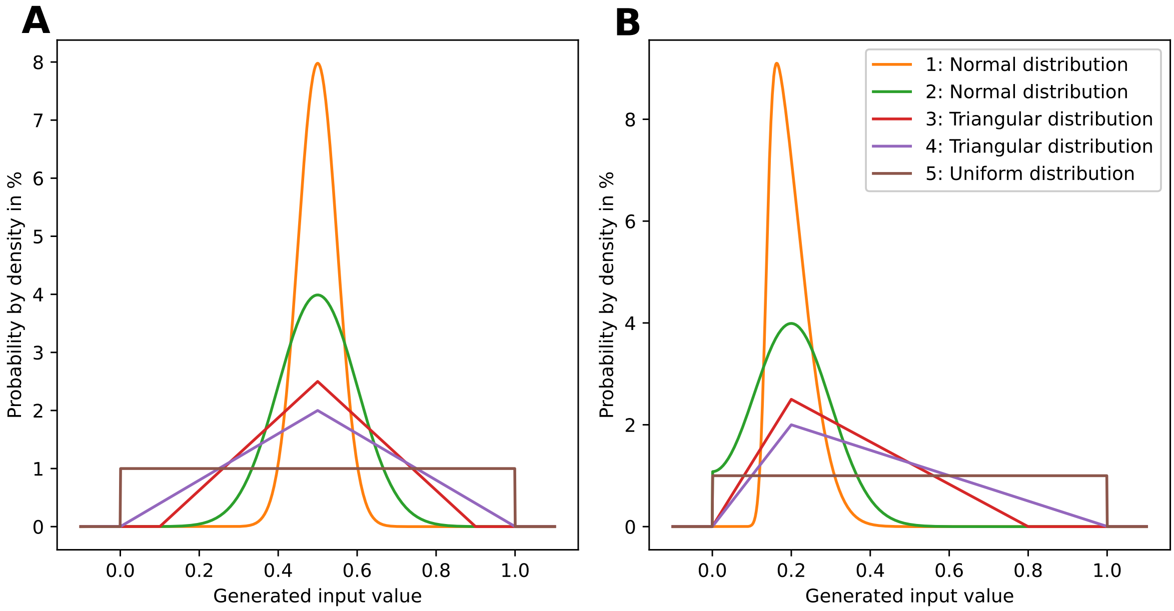

Figure 2.7: Distribution of initial inflow, transfer coefficients, and efficiencies for (a) an input value of 0.5 and (b) an input value of 0.2

The skew factor a of these two distributions was determined empirically. The target was, to keep the value of the probability density function of the skewed normal distribution ($\mathcal{S}$ for $x = 0$ smaller or equal to the value or the original normal distribution for $\mu = 0.5$ at $x = 0$, which is a value very close to 0 [1]:

$$\mathcal{S}(x = 0|\mu, \sigma^2 = 0.05^2, a) \leq \mathcal{N}(x = 0|\mu = 0, \sigma^2 = 0.05^2) \tag{2.2}$$

In order to avoid a numerical approximation of a for each input, it was approximated by a linear function once the boundary values were determined. The boundary for the location of the skewed normal distribution (see SciPy, 2022) for the uncertainty score 1 are 0.05 and 0.95, and 0.1 and 0.9 for the uncertainty score 2. It was found that the skew factor a becomes extremely large beyond those boundaries. Therefore, the skewed normal distribution is replaced by a folded normal distribution which avoids this unwanted behavior. This can be seen in Figure 2.7 B for the uncertainty score 2 (green line). Although, the peak of the folded distribution changes, it needs to be disclaimed that the mean of the distribution does not necessarily match the actual input.

The behavior of the triangular distributions is less complicated. The distribution for the uncertainty score 4 moves symmetrically along the x-axis until its corner reaches either 0 or 1 (see Figure 2.8).

[1] Equation 2.2 holds true for the distribution for the uncertainty score 1, for uncertainty score 2 σ has to be changed to $\sigma^2 = 0.1^2$

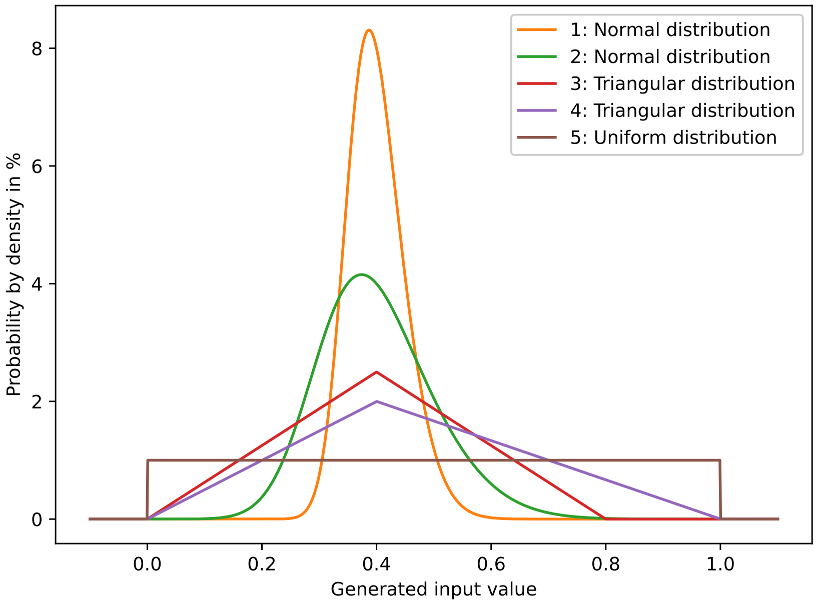

Figure 2.8: Distribution of initial inflow, transfer coefficients, and efficiencies for an input value of 0.4

Once this happens, the peak of the triangular distribution is set to the location of the original input value. This is also the general behaviour of the triangular distribution assigned to inputs with the uncertainty score 4 (see Figure 2.7 B and 2.8)

Examplary histograms of the resulting input distributions are shown in Appendix C. As those examples show, not all histograms follow the defined distribution. This is due to the fact that transfer coefficients which define the forking of one flow have to sum up to 1. This way, mass conversation is insured. This is done after the random numbers are generated. It is necessary to generate a numbers for all transfer coefficients to see the contribution to uncertainty of each single input.

2.4.3. Evaluation of Monte Carlo Simulations

The results of the Monte Carlo simulations which are going to consist of the results of $n = 10,000$ individual runs are going to be used to attribute the uncertainty in the model to the inputs and to perform a sensitivity analysis following the example of Fishman et al. (2018). The first step in the evaluation is to find the correlation between all inputs and one or several selected outputs (e.g. the total use stock). Although, the Pearson correlation obtains more precise results, it cannot be used because not all of the inputs are normally distributed (see above) which is a necessary condition. Therefore, the Spearman rank correlation is used (Gauthier, 2001). Therefore, the inputs have to be ranked as presented in the following table:

	Input		Result						
			Year 0			...	Year 35		
	Value	Rank	Value	Rank	d	...	Value	Rank	d
run 1	0.89	2	0.65	3	1		0.69	1	-1
run 2	0.85	3	0.66	2	-1		0.68	2	-1
⋮	⋮	⋮	⋮	⋮	⋮		⋮	⋮	⋮
run 1000	0.91	1	0.72	1	0		0.63	3	2

Table 2.5: Example Monte Carlo inputs and results including value and rank

The highest value receives the rank 1, the next largest value receives the rank 2, and so on. In the following equations, inputs are represented by a and results by b, and the index i represents inputs, the index r represents runs, and the index j represents years. To obtain the correlation, the difference between the ranks of the input and the results have to be calculated (Cao et al., 2018):

$$d_{irj} = b_{irj} - a_{ir} \tag{2.3}$$

It is important to recognize, that the results change with each year while the input of the model stays constant. Using d, the Spearman's rank-correlation coefficient can be calculated where n is the number of runs (Cao et al., 2018):

$$\rho_i j = \frac{1 - 6\sum_{r=1}^{n} d_{irj}^2}{n^3 - n} \tag{2.4}$$

On this basis, the uncertainty contribution of each input regarding the selected output can be calculated. This is expressed by the normalized squares of the Spearman's rank-correlation coefficients (Cao et al., 2018):

$$C_i = \frac{\rho_j^2}{\sum_{i=1}^{n} \rho_{ij}^2} \tag{2.5}$$

So, C_i represents the relative contribution of an input to the variance of the considered result (uncertainty) (Cao et al., 2018).

3
Data

This chapter describes the origin of the used data. Assumptions were made since existing data sets were extended and data on reuse is scarce. In the attempt to explicitly point out all assumptions, they were highlighted in italic.

3.1. Data as present in the models

The used MaTrace model of Godoy León et al. (2020) takes the year 2015 as initial input year. Considering the eventful history of recent years and the mentioned drivers influenced by climate mitigation policies, it is fair to assume that the situation has changed drastically (in the year 2022). However, the choice of the initial input year is based on the previous work of the researchers.

Godoy León and Dewulf (2020) developed a framework to assess the quality of collected data and applied the framework on cobalt. Therefore, they consulted over 330 sources and withdraw data from 76. Each obtained value received a Data Quality Rating (DQR) which is based on four to five criteria. Based on this research, the most reliable data was selected to conduct the MaTrace model (Godoy León et al., 2020).

The data used for the reuse model is withdrawn from the work of Glöser-Chahoud et al. (2019) who applied the model of Thiébaud et al. (2017) on Europe. Since they use the year 2015 as the initial year as well, the data of both models is compatible regarding temporal and regional scope. The data set which combines the data from Godoy León et al. (2020) and Glöser-Chahoud et al. (2019) will be referred to as **Combined Data Set** in the following.

3.2. Extending reuse data

The reuse model of Glöser-Chahoud et al. (2019) tries to cover consumer electronics in Europe by considering smartphone, mobile phones, tablets and laptops. Although these devices cover the largest share, they do not cover the whole landscape of devices requiring portable batteries. Furthermore, it poses a rather homogeneous group regarding their lifetime distributions. In order to add diversity, I decided to extend the data by three additional categories: cordless power tools, E-bikes and others. This extended data set will be referred to as **Extended Data Set** in the following. The distribution of the initial inflow will base on Pillot (2012) who provides the market share of different devices in MWh battery capacity. *It is assumed that the proportional capacity reflects the relative cobalt content.*

Cordless power tools are used by professionals and consumers this includes tools such as drills and saws, as well as gardening tools such as mowers and hedge trimmers (Union, 2006). Cordless household tools will be considered in the same category.

The category Others will entail less significant electronics such as MP3 players, cameras and toys.

3.3. Data on E-bikes

Currently, data on E-bikes is scarce, contemporary studies focus on customers who recently bought an E-bike and not on long term ownership patterns (Fyhri & Beate Sundfør, 2020). Additionally it needs to be considered, that data regarding the use and reuse of E-bike batteries needs to be derived and not necessarily data on E-bikes themselves.

The only hard data available is the average ownership time of a bicycle, 8.3 years (Balton, 2022) and the average lifetime of an E-bike battery which is 4.12 years (with an Weibull shape of 4.34) (Guo et al., 2021). This means, that an E-bike owner will most likely use multiple batteries throughout the lifetime of a bike. *I assumed that this circumstance leads to a decreased probability for E-Bike batteries to be reused. Therefore it is assumed that a total of 10% of firstly used batteries will be reused.*

Regarding the share of devices entering the hibernating stock, it is considered, that size plays an important role. Small items are more likely to be stored than large items (Thiébaud (-Müller) et al., 2018). *Since there is data on TV hibernation (Thiébaud et al., 2017) and since a TV is the device which comes closest in size of all available ones to an E-bike battery, I assumed that E-bike batteries are hoarded to the same extent as TVs.*

Those assumptions inspired the transfer coefficients as presented in Table 3.1.

From	To	Coefficient
First service life	Secondary use	0.07
	First storage	0.22
	Disposal	0.71
Second service life	Tertiary use	0.03
	Second storage	0.26
	Disposal	0.71
Third service life	Third storage	0.29
	Disposal	0.71
First storage	Secondary use	0.14
	Disposal	0.86
Second storage	Tertiary use	0.7
	Disposal	0.93

Table 3.1: E-Bike transfer coefficients

The estimated lifetime of E-bike batteries are known and the assumption is established that only few batteries are going to be reused. *Therefore, the given average lifetime is assumed for the first use. The Weibull scale is diminished to account for batteries leaving the stock and which are reused.*

The lifetime for the second use is the same since it is assumed that customers buying E-bike batteries second hand have a higher tolerance towards a diminished capacity. The third average service lifetime is set to 2 years. *This is based on the underlying assumption that batteries may not be fit for purpose very long once they enter their third service life.*

The hibernating times are made up based on the assumption that storage times of perishable products should not be longer than their service time. The Weibull shapes are assumed to be the same ones as for TVs.

	Mean lifetime	Weibull shape
First service life	4.12	3
Second service life	4.12	2.5
Third service life	2	1.5
First storage	2	1.7
Second storage	1.5	1.59
Third storage	1.5	1.59

Table 3.2: E-Bike lifespans

3.4. Data on cordless power tools

The estimated lifetime of batteries used in cordless power tools was found to be 10 year (Mudgal et al., 2011). *Therefore, i assumed that in private ownership the lifetime of the tool exceeds the lifetime of the battery. Based on this I assumed that most batteries go to disposal, few to storage and only little to reuse.*

The following transfer coefficient table is based on those assumptions.

From	To	Coefficient
First service life	Secondary use	0.05
	First storage	0.15
	Disposal	0.8
Second service life	Tertiary use	0.02
	Second storage	0.2
	Disposal	0.78
Third service life	Third storage	0.3
	Disposal	0.7
First storage	Secondary use	0.1
	Disposal	0.9
Second storage	Tertiary use	0.05
	Disposal	0.95

Table 3.3: Cordless power tools transfer coefficients

Regarding the Weibull shape of the lifetime it is set to be 1.5 for the first service life while it is smaller for the followings based on assumptions hereafter. *There are high frequency equipment users and others who use it only rarely. Hence there is a discrepancy in lifetime among users. To model this, the Weibull scale was reduced considering earlier failures. The storage periods are assumed to be longer than for E-bikes, since it is assumed that tool owners have more space to store EOL products.*

	Mean lifetime	Weibull shape
First service life	9	1.5
Second service life	5	1.2
Third service life	2	1.1
First storage	3	1.7
Second storage	2	1.59
Third storage	2	1.59

Table 3.4: Cordless power tools lifespans

3.5. Data on other cordless electronics

The category Others includes e.g., cameras, mp3 players, and similar devices. *I assumed that those devices are rather small and easy to store when they reached their EOL. Following this, I assumed that they follow the use and storage behaviour of mobile phones as described by Thiébaud et al. (2017).*

Transfer coefficients

From	To	Coefficient
First service life	Secondary use	0.05
	First storage	0.15
	Disposal	0.8
Second service life	Tertiary use	0.02
	Second storage	0.2
	Disposal	0.78
Third service life	Third storage	0.3
	Disposal	0.7
First storage	Secondary use	0.1
	Disposal	0.9
Second storage	Tertiary use	0.05
	Disposal	0.95

Table 3.5: Others electronics transfer coefficients

The same assumption is applied to the lifetimes.

	Weibull scale	Weibull shape
First service life	3.27	2.13
Second service life	3.59	2.17
Third service life	3.59	2.17
First storage	2.16	1.17
Second storage	3.9	1.46
Third storage	3.9	1.46

Table 3.6: Others electronics lifespans

4

Results

In this chapter the results of the research will be presented following the order outlined in the methodology chapter (see Chapter 2 Methodology). First, the general model output will be described (see Section 4.1). As the model is largely based on the work of other authors, this is followed by the results of the impact analysis. I will present how the model and data extension alter the most important measure - the total in-use stock (see Section 4.2.1). After this, the altered model (the Reuse-MaTrace mode) and data set (the Extended Data Set) will be used for all further experiments. Also for the second part of the impact analysis displaying the impact of adding a second and a third use cycle to the system (see Section 4.2.2). The last part of this chapter covers the results of the Monte Carlo Simulations which give insight into the uncertainties of the model inputs (see Section 4.3).

4.1. General model output

In this section, the general model output is described which refers to the model as it was presented in Section 2.1 and Section 2.2 using Extended Data Set as it was described in Chapter 3. The general model output is best described by the following figure because it represents the stocks and accumulated outflows. This means that it displays the fate of the in-flowing cobalt in 2015 over the course of the next 35 years.

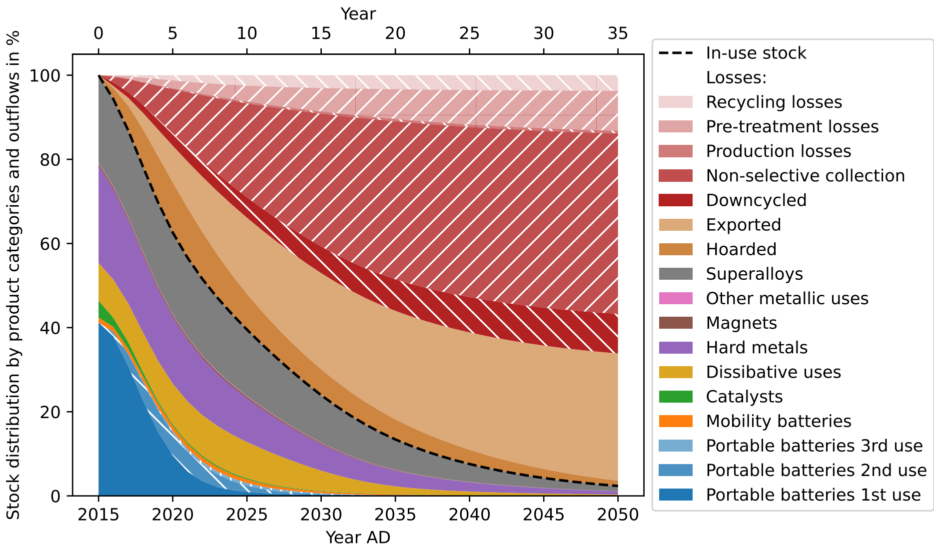

Figure 4.1: Distribution of stocks and and accumulated outflows based on the cobalt inflow in 2015. The black dashed line marks the total in-use stock. Areas in red with white stripes mark losses. First, second and third use of portable batteries is represented by different shades of blue.

The figure is an area chart in which stocks and accumulated outflows are stacked on top of each other. The top layer always reaches 100 % which indicates that the graph covers all outflows considered in the model. The red dashed line illustrates the percentage of the material which can be found in the in-use stock. All areas below this line represent the in-use stock of the different product categories. The product category *Portable batteries* is broken down into first, second, and third use since this is the product category on which the reuse model was applied (see Figure 4.2 for breakdown into products).

The black areas with white stripes represent losses. Downcycling refers to the conversion of metals and alloys to stainless steel (also see Section 2.1 and Godoy León et al. (2020)) and is considered to be a loss. The two areas in between are hibernating stocks and exports. Those are not part of the in-use stock nor the losses since exported materials and goods have the potential to be reused within another geographical scope. The same holds true for hibernating stocks.

Figure 4.1 allows to draw conclusions regarding the overall dynamic of the model in combination with the used data. Looking at the losses, it is apparent that non-selective collection makes up by far the largest share of the losses (about 43 % of the former inflow in 2050) while recycling losses (pre-treatment and recycling itself) account for only about 13 % of the former inflow in 2050. Production losses appear to be very small in comparison.

Looking at exports and hibernating stocks it can be seen that hibernating stocks build up in the beginning and slowly vanish towards the year 2050. The area of exports is constantly increasing until it becomes, with about 30 %, the second largest in 2050.

Regarding the stocks of in-use product categories, it can be seen that most stocks deplete constantly. *Dissipative uses* are the only exception from that behaviour, they make up 9 % of the inflowing material in the year 2015 and the stock increases until it peaks with 9.8 % in the year 2021. It depletes from there onwards and it can be observed that the stock of portable batteries depletes comparatively quick until it is almost vanished in the year 2030. Although, the secondary in-use stock of *portable batteries* covers a clearly visible area it is important to recognize that the stock of portable batteries experiencing a third use-cycle can barely be seen.

Figure 4.2 was created in order to investigate the dynamic of the *portable batteries* stock. It is an area chart displaying the in-use stock of the *portable batteries* split up in products and use cycles.

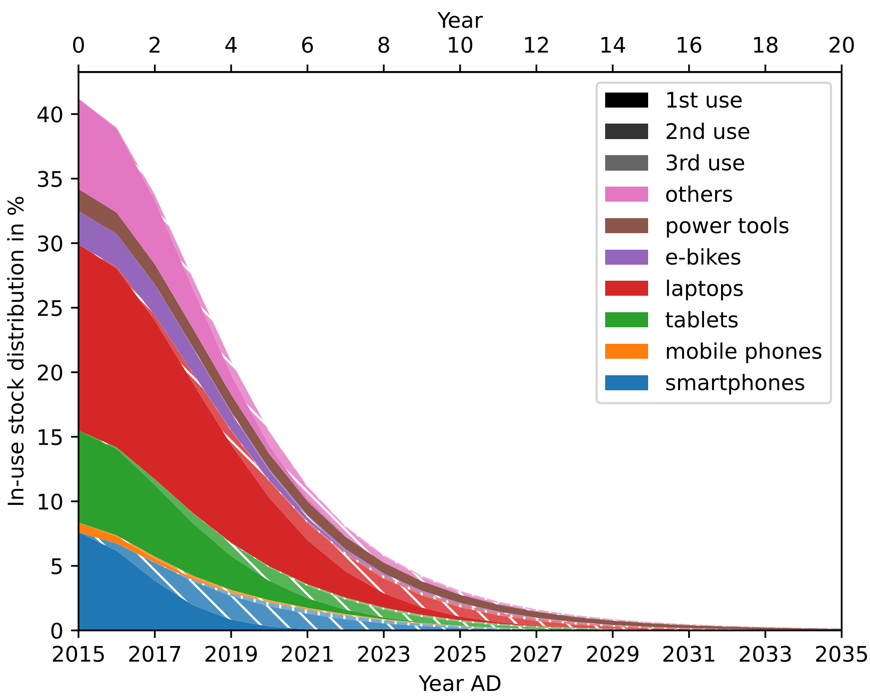

Figure 4.2: Distribution of the in-use stock of portable batteries among products of the Reuse-MaTrace model using the Extended Data Set which consists of the data of Godoy León et al. (2020), Glöser-Chahoud et al. (2019), and other collected data (see Chapter 3). The individual use cycles are separated by texture and saturation.

Besides the general stock distribution over products, several observations can be made. Firstly, it can be seen that the second use phase holds significant shares for some product groups such as smartphones and tablets. For other product groups such as power tool and e-bike batteries, the share of the second use-phase is barely visible which is in line with the assumptions made in Chapter 3. Furthermore, the share of the products in their third use phase can only be seen when zoomed in. This observation gave the impulse to closer investigate the impact of the consideration of multiple use cycles (for results see Section 4.2.2).

4.2. Impact analysis

In the following, I will investigate what impact it has to incorporate the reuse model into the existing MaTrace model as created by (Godoy León et al., 2020). I explained in Section 2.3, that I will investigate how the total in-use stock changes. First I will focus at the changes when the reuse model is integrated into the MaTrace model (considering Combined Data Set and Extended Data Set), and secondly, on how much the second and third use cycle add to the total in-use stock.

In order to put the deviation into perspective I decided to compare the points in time when the total in-use stock hold 75%, 50%, and 25% of the inflow in 2015.

4.2.1. Model extension

As outlined above, the first impact to investigate is the extension of the MaTrace model by Godoy León et al. (2020) by the reuse model. Figure 4.3 displays (a) the total in-use stock and (b) the in-use stock of *portable batteries* of the MaTrace model by Godoy León et al. (2020) and the Reuse-MaTrace model using Combined Data Set and Extended Data Set. The vertical lines mark the instances in time when the in use-stock holds 75 %, 50 %, and 25 % of the in-use stock.

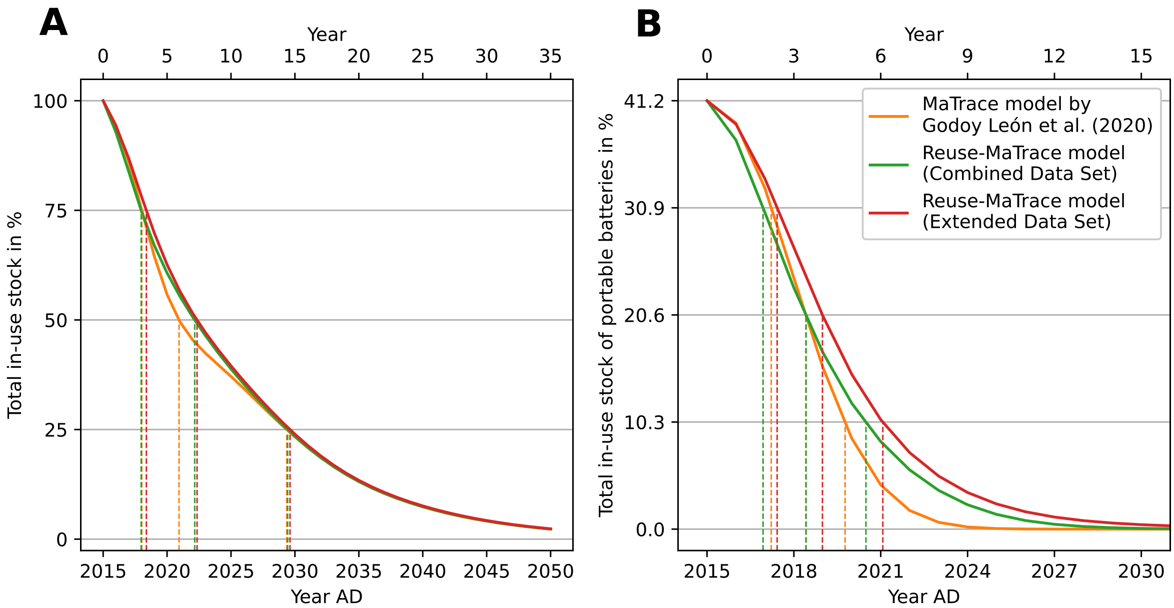

Figure 4.3: Comparison of the total in-use stock (a) and the portable batteries in-use stock (b) of the MaTrace model by Godoy León et al. (2020), the Reuse-MaTrace model using the Combined Data Set (green line, consisting of data of Godoy León et al. (2020) and Glöser-Chahoud et al. (2019)), and the Reuse-MaTrace model using the Extended Data Set (red line, the data set includes additional products for the product category portable batteries, see Chapter 3). The vertical lines marks the time when the representative stock holds only 75 %, 50 %, and 25 % of the initial inflow.

Table 4.1 holds the stock depletion instances regarding the total in-use stock (as in Figure 4.3 A).

Instant when the in-use stock is depleted to:	75 % Year	75 % Deviation	50% Year	50% Deviation	25 % Year	25 % Deviation
MaTrace model by Godoy León et al. (2020)	2018.0	0.0	2020.9	0.0	2029.4	0.0
Reuse-MaTrace model (Combined Data Set)	2018.0	0.0	2022.2	1.3	2029.4	0.0
Reuse-MaTrace model (Extended Data Set)	2018.4	0.4	2022.4	1.5	2029.6	0.2

Table 4.1: Comparison of instant of total in use-stock depletion by models and data sets. The decimal digits represent fractions of years (not months). The deviations are based on the instances when the MaTrace model by Godoy León et al. (2020) is considered. The Combined Data Set consists of data of Godoy León et al. (2020) and Glöser-Chahoud et al. (2019). The Extended Data Set includes additional products for the product category portable batteries (see Chapter 3).

The figure and the table above display, that the deviation of stock-depletion instances regarding the total in-use stock are very small at 75 % and 25 % (less than 0.5 years in both cases). At 50 % the deviation from the MaTrace model by Godoy León et al. (2020) to the Reuse-MaTrace model using Combined Data Set is 1.3 years and to the Reuse-MaTrace model using Extended Data Set 1.5 years.

These findings lead to the conclusion that the modeling changes do not impact the total use-stock in all instances to the same extent. Figure 4.4 A displays the relative stock deviation of the Reuse-MaTrace model using Combined Data Set and Extended Data Set in comparison to the MaTrace model by Godoy León et al. (2020). The orange lines represent the instances when the total in-use stock of the MaTrace model by Godoy León et al. (2020) holds 75 %, 50 %, and 25 %.

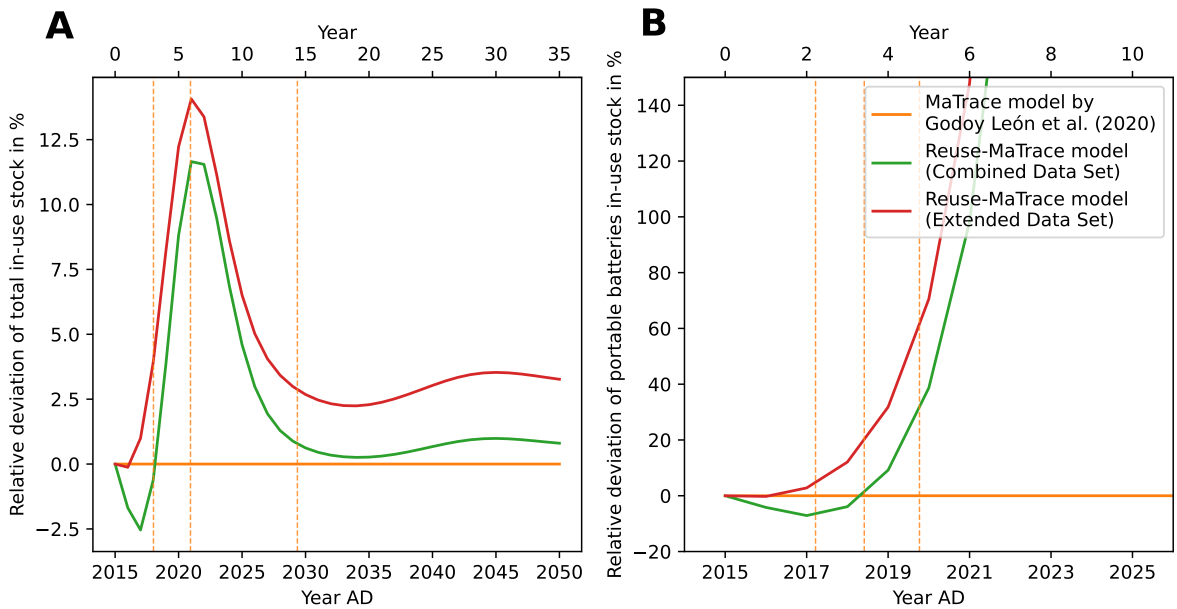

Figure 4.4: Relative comparison of the total in-use stock (a) and the portable batteries in-use stock (b) of the MaTrace model by Godoy León et al. (2020) (orange line), the Reuse-MaTrace model using the Combined Data Set (green line, consisting of data of Godoy León et al. (2020) and Glöser-Chahoud et al. (2019)), and the Reuse-MaTrace model using the Extended Data Set (red line, the data set includes additional products for the product category portable batteries, see Chapter 3). The vertical, orange lines mark the instances in time when the stock of the MaTrace model by Godoy León et al. (2020) holds only 75 %, 50 %, and 25 % of the initial inflow (see Figure 4.3).

It can be seen, that both lines peak in the year 2021, which is the instance when the total in-use stock of the MaTrace model by Godoy León et al. (2020) is depleted to 50 %. At this instance, the total in-use stock of the Reuse-MaTrace model using the Combined Data Set is about 13 % larger and when the Extended Data Set is applied it is about 11.5 % larger. Additionally, it can be seen that the total in-use stock of the Reuse-MaTrace model using the Extended Data Set is constantly above 0, while the line for the Combined Data Set goes goes below 0 in the very beginning. Therefore, I concluded that the total in-use stock over all increased for all instances when the MaTrace model by Godoy León et al. (2020) is extended (the following section will discuss the actual impact of the consideration of multiple use cycles).

Looking at Figure 4.3 B it can be seen that the stock behaviour of the different models is different when only the in-use stock of portable batteries is considered. In contrast to the total in-use stock, all lines are distinguishable from the very beginning and their deviation becomes larger till the point when the in-use stock of portable batteries of the MaTrace model by Godoy León et al. (2020) is almost depleted. Table 4.2 gives the instances when the potable batteries in-use stock of each model has decayed to 75 %, 50 %, and 25 %.

Instant when the in-use stock is depleted to:	75 % Year	75 % Deviation	50% Year	50% Deviation	25 % Year	25 % Deviation
MaTrace model by Godoy León et al. (2020)	2017.2	0.0	2018.4	0.0	2019.8	0.0
Reuse-MaTrace model (Combined Data Set)	2016.9	-0.3	2018.4	0.0	2020.5	0.7
Reuse-MaTrace model (Extended Data Set)	2017.4	0.2	2019.0	0.6	2021.1	1.3

Table 4.2: Comparison of instants of portable batteries in-use stock depletion by models and data sets. The decimal digits represent fractions of years (not months). The deviations are based on the instances when the MaTrace model by Godoy León et al. (2020) is considered. The Combined Data Set consists of data of Godoy León et al. (2020) and Glöser-Chahoud et al. (2019). The Extended Data Set includes additional products for the product category portable batteries (see Chapter 3).

The stock of all models reaches 75 % within a instant deviation of 0.5 years. When the stock decays to 25 % it is already at 1.3 years. This difference is also reflected in Figure 4.4 B. It can be observed, that the relative portable batteries in-use stock deviation for both data sets is increasing steeply, after the line considering the Reuse-MaTrace model using the Combined Data Set reaches its minimum in 2017. Although, I am tempted to say, that the portable batteries stock increases almost exponentially when reuse is considered in the model, the underlying reason for this behaviour needs to be understood. After the year 2024 the portable batteries in-use stock of the MaTrace model by Godoy León et al. (2020) is almost 0. Therefore, the values of the other models are many times larger which is why a relative comparison is misleading in this case.

In conclusion I found that the total in-use stock as well as the portable battery in-use stock becomes larger when reuse is considered in the modeling process. The following section illustrates the impact of considering a second and a third use cycle.

4.2.2. Use cycle impact

This subsection presents the results of the impact analysis regarding the consideration of multiple use cycles. As explained in Section 4.2.2, this analysis is based on the Reuse-MaTrace model applying the Extended Data Set. The model was run, once considering only one use-cycle of portable batteries. The results of this run were then used as a benchmark in the following. Then the model run considering two use cycles and finally three use cycles. Those consecutive runs created the results represented here.

Figure 4.5 A displays the total in-use stock and B the in-use stock of portable batteries of the Reuse-MaTrace model using the Extended Data Set considering one, two, and three use-cycles of for products within the *portable batteriers* product category. The vertical lines mark the instances in time when the in use-stock holds 75 %, 50 %, and 25 % of the in-use stock.

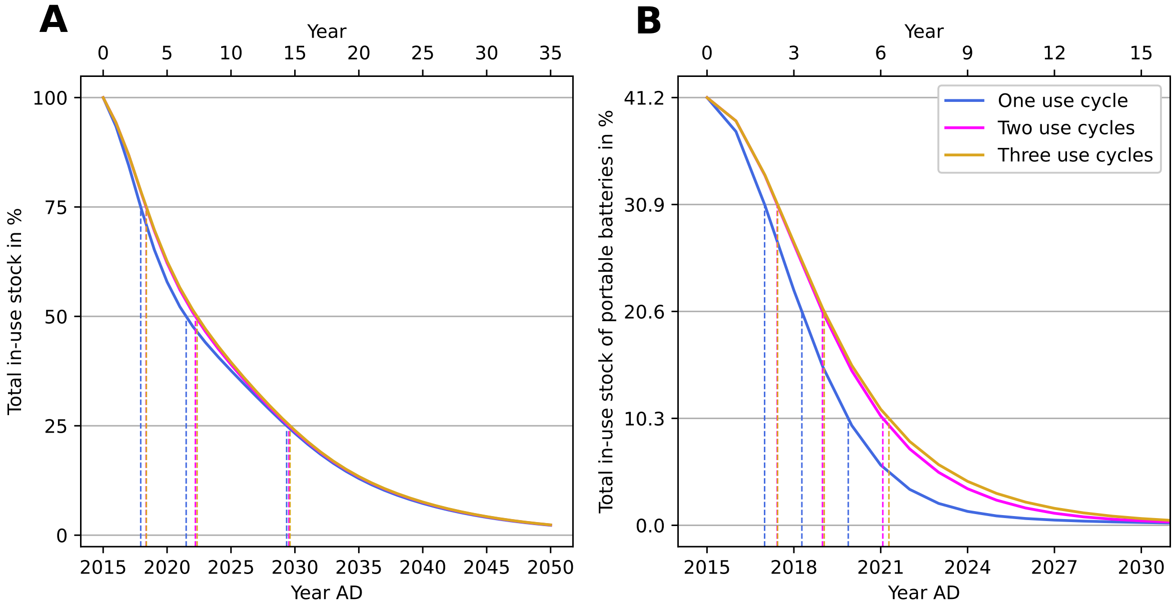

Figure 4.5: Comparison of the total in-use stock (a) and the portable batteries in-use stock (b) of the Reuse-MaTrace model when one use cycle (blue line), two use cycles (magenta line), or three use cycles (golden line) are considered. The vertical lines mark the instances in time when the representative stock holds only 75 %, 50 %, and 25 % of the initial inflow.

Focusing on the total in-use stock (Figure 4.5 A) shows, that only the lines for one and three use cycles are clearly distinguishable, since the line representing three use cycles appears to cover the line representing two use cycles. This is also reflected in Table 4.3 which displays the instances when the total in-use stock holds 75 %, 50 %, and 25 %. The instances when three use-cycles are considered are always 0.1 years larger.

Instant when the	75 %		50%		25 %	
in-use stock is depleted to:	Year	Deviation	Year	Deviation	Year	Deviation
One use cycle	2018.5	0.0	2021.5	0.0	2029.4	0.0
Two use cycles	2018.9	0.4	2022.2	0.7	2029.5	0.1
Three use cycles	2019.0	0.5	2022.3	0.8	2029.6	0.2

Table 4.3: Comparison of instant of total in use-stock depletion by number of use cycles. The decimal digits represent fractions of years (not months). The deviations are based on the instances when only one use cycle was considered.

The deviation of instances is the largest in the column presenting the instances for 50 % stock depletion. So, it can be assumed that the impact of considering additional use-cycles for *portable batteries* is the largest between the instant when the in-use stock holds 75 % and the instant when it holds 25 %. This assumption gets confirmed by analysing Figure 4.6. The figure displays the relative stock deviation of the results considering two and three use-cycle in comparison to the results when only one use-cycle was considered. Figure 4.6 A displays the deviation of the total in-use stock where the orange lines represent the instances when the total in-use stock holds 75 %, 50 %, and 25 % when only one use cycle is considered.

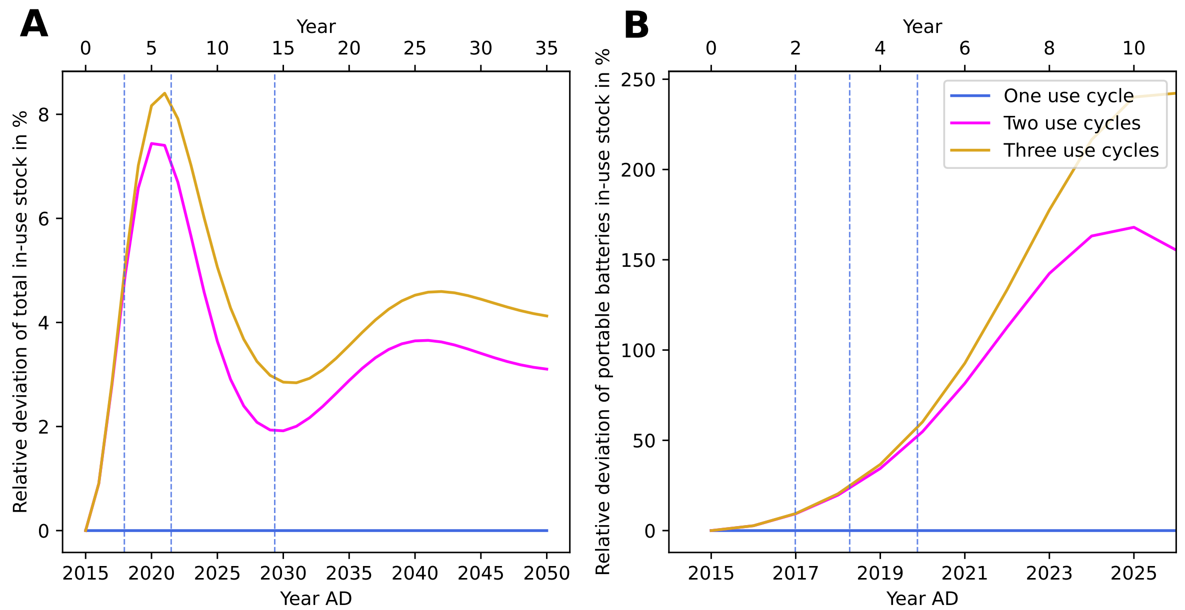

Figure 4.6: Relative comparison of the total in-use stock (a) and the portable batteries in-use stock (b) when one use cycle (blue line), two use cycles (magenta line), or three use cycles (golden line) are considered. The vertical, blue lines mark the instances in time when the stock of the Reuse-MaTrace model which considers only one use cycle holds only 75 %, 50 %, and 25 % of the initial inflow (see Figure 4.5).

As it can be seen, both lines peak around the instance when the in-use stock is depleted by 50 %. In this peak, the total in-use stock is about 8.5 % larger when three use-cycles are considered and about 7.5 % larger when only two use-cycles are considered. Hence, considering the additional third use-cycle results in an stock increase of 1 % which proofs that it does make a difference even though this was not visible in Figure 4.5.

Focusing on the in-use stock behaviour of the *portable batteries* product category I found an overall similar behaviour as for the previous impact analysis (see Section 4.2.1). Looking at Figure 4.5 B one finds that the lines representing two and three use-cycles deviate early on from the line which represents one use cycle. This deviation increases until the line representing one use-cycle starts to approach 0 % around the year 2022. This behaviour is also reflected in Table 4.4. The table gives the instances when the potable batteries in-use stock of each considered case has decayed to 75 %, 50 %, and 25 %. The deviation between the portable battery stock for the case when one use-cycle and when three use-cycles are considered is the smallest when 75 % of the initial stock is still in use and the largest when only 25 % are left in use.

Instant when the in-use stock is depleted to:	75 % Year	75 % Deviation	50% Year	50% Deviation	25 % Year	25 % Deviation
One use cycle	2017.2	0.0	2018.3	0.0	2019.9	0.0
Two use cycles	2017.7	0.5	2019.0	0.7	2021.1	1.2
Three use cycles	2017.8	0.6	2019.0	0.7	2021.3	1.4

Table 4.4: Comparison of instant of portable batteries in-use stock depletion by number of use cycles. The decimal digits represent fractions of years (not months). The deviations are based on the instances when only one use cycle was considered.

When looking at Figure 4.6 B, the relative deviation of the portable batteries in-use stock behaves similarly to the previous impact analysis (see Section 4.2.1, Figure 4.6). The steep growth in deviation can be explained by the fact, that the in-use stock when one use cycle is considered converges earlier to 0 the in the two other cases.

4.3. Monte Carlo simulations

Section 2.4 discussed that the purpose of the Monte Carlo simulations and the analysis of the results is to find the inputs which insert the greatest uncertainty into the model. This is measured with C (see equation 2.5), the relative contribution of an input to the variance of the considered results. The variance of the results is introduced by the randomization of the inputs before each run. Therefore, it is important to be aware of the variance of the regarded result at each time since the relevance of a high C-value vanishes when the variance in the model is very small. The result I deemed to be the most relevant is the total in-use stock, since this is the most relevant measure regarding the resource efficiency of materials, in this case cobalt.

Figure 4.7 displays the variance of the total in-use stock represented by several confidence bands. Those bands base on quantiles. A quantile is calculated by arranging the results in ascending order (e.g. the in-use stock of all runs in the year 2025). Considering that the Monte Carlo simulations contain 10,000 runs, the 1 % quantile would be the 100th value of those ordered result. Hence, a confidence band covers 98 % of all values between the 1 % quantile and the 99 % quantile. The wider the confidence bands, the larger the variation in the results.

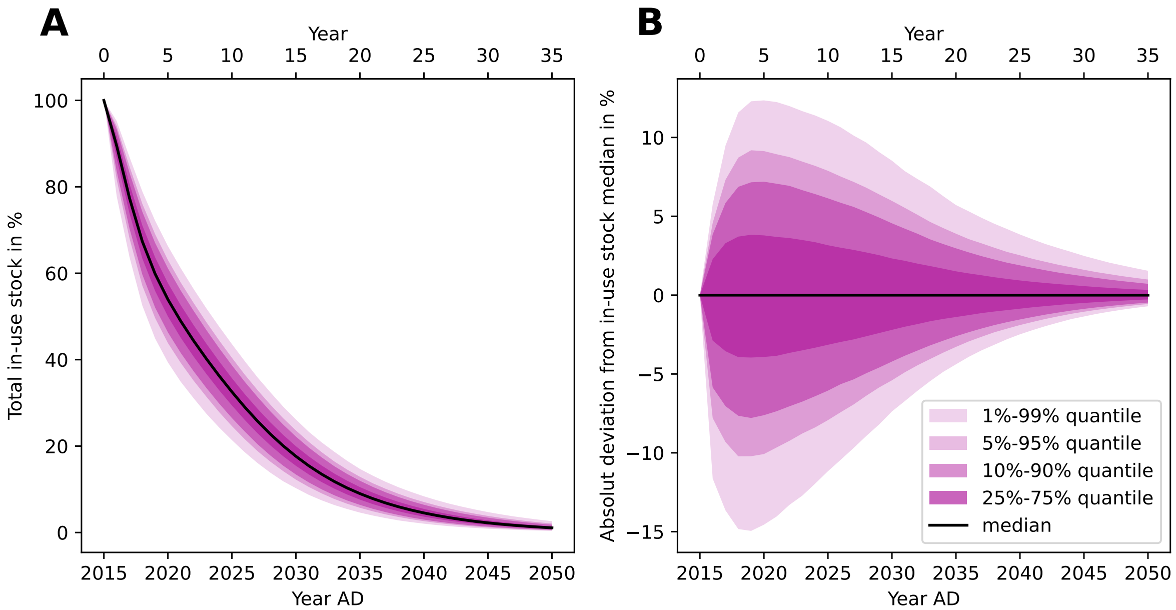

Figure 4.7: Confidence bands of the total in-use stock derived from Monte Carlo simulations (a) and the absolute deviation of the confidence bands from the median of the total in-use stock (b)

As the figure shows, there is no variation in 2015 because all models start with an inflow of 100 %. The confidence bands are especially wide between the years 2018 and 2020 (see Figure 4.7) and become constantly narrower until the variance is very small in the year 2050. This alternation in variance is important to consider in the following course. Besides the variation, the actual in-use stock size is important to consider, if the stock is almost depleted in the year 2050, it is not expediently to discuss which input inserts the most uncertainty into the model at this point in time. For this reason, the following graphs contain a line indicating the total in-use stock (dashed red line) and a line indicating the 1 % to 99 % quantile uncertainty bandwidth (solid purple line). Here the bandwidth is defined as the absolute difference between the 1 % quantile and the 99 % quantile per instance.

Figure 4.8 displays the relative contribution of the inputs to the variance (in the following uncertainty) of the total in-use stock. The uncertainties of the inputs are summed by input vector (e.g. the sum of the contribution of all recycling efficiencies instead of the contribution of recycling efficiency for portable batteries, mobility batteries etc.).

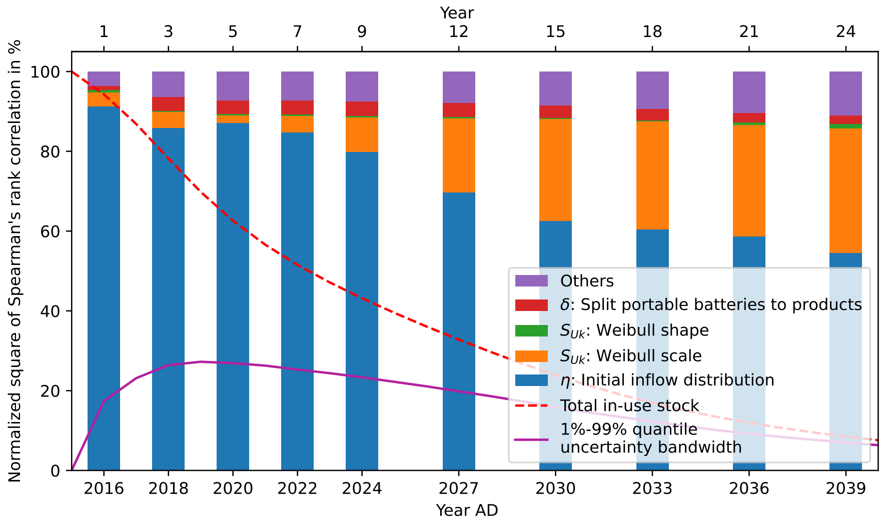

Figure 4.8: Share of uncertainty in total in-use stock by input vectors. The dashed red line represents the total in-use stock and the solid purple line represents the 1 % to 99 % quantile uncertainty bandwidth as measure for the uncertainty present at the regarded instances.

The year 2015 is not represented since no uncertainty is present as explained, which can also be seen in Figure 4.7 B. From 2016 onward, the most important contributor is η the distribution of the initial inflow. Despite its decline it is deemed the most important one since it is especially strong, when the total in-use stock is still high (consider the vertical lines in the graph) and when the variation (solid purple line) in the total in-use stock is largest.

The second most important contributor is the Weibull scale of the in-use stock for all product categories except *portable batteries* (all product categories where reuse is not considered). The lifetimes of the larger share of the material is determined by this input, thus it is intuitive that it contributes to the uncertainty in the system which also explains its increased importance. Most Weibull shapes β are larger than 1 which means that the survival rate in the first few years is high (also see Figure 2.5). The Weibull scale affects the point in time when the failure rate increases. Therefore, the contribution to the uncertainty of these Weibull scales increase over time. Far less relevant are the next largest contributors, Weibull shapes connected to the mentioned Weibull scales and the split of the material in portable batteries over product δ. The contribution of the Weibull shape only becomes considerably large after 2040, therefore, I will not discussed or considered it any further. At this point in time the largest share of the stock is already depleted and the variation in the results is small in this period (see Figure 4.7). Looking at the data (see Appendix A) it is explainable why δ holds some uncertainty. Products have different lifetimes and transfer coefficients from a use phase to the next use phase and from hibernating stocks to the next use phase. Some products have configurations which contribute more to resource efficiency than others, to me it makes sense to see this reflected in the mapping of uncertainties.

Since the main contributor η is significantly more impact full than all other inputs, it will be investigated more closely. Figure 4.9 displays the uncertainties of the components of the vector η (material share allocated to product category) ignoring all other sources of uncertainty.

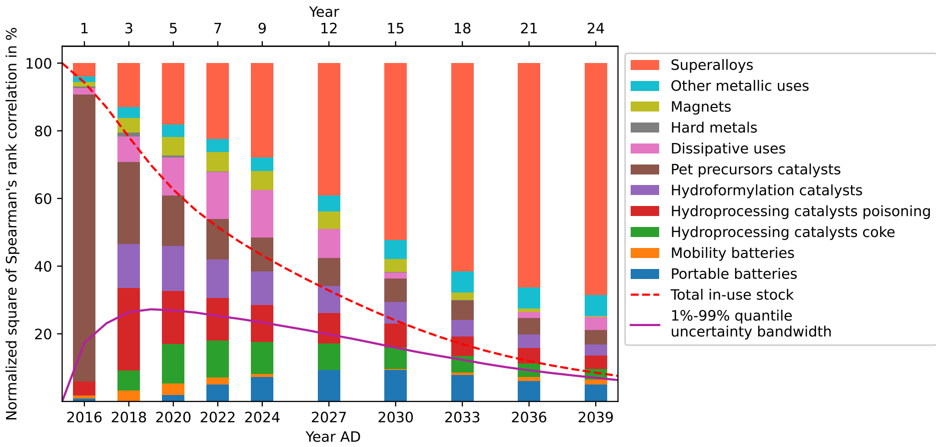

Figure 4.9: Share of uncertainty in total in-use stock by the split of the initial input over product categories. The dashed red line represents the total in-use stock and the solid purple line represents the 1 % to 99 % quantile uncertainty bandwidth as measure for the uncertainty present at the regarded instances.

Looking at the graph, some observations can be explained by consulting the input data while some cannot. The most obvious detection is the increasing contribution of the initial share of superalloys to the uncertainty of the total in-use stock. This is the product category with the longest expected lifetime. Therefore, it is understandable that its share introduces uncertainty in the long run when all other stocks are almost depleted. The same applies for the category pet precursors catalysts, the category with the shortest lifetime. Hence, its share of the initial inflow determines the size of the total in-use stock especially in the beginning. Other phenomena cannot be explained. For example the two occurrences of dissipative uses. At this point I have to admit that the model might be too complex to fully comprehend its dynamics and that I cannot fully explored them within the scope of this thesis.

In order to learn more about inputs having a smaller but considerable impact on the total in-use stock, new C-values were calculated factoring out the three largest contributes. The results are presented in Figure 4.10.

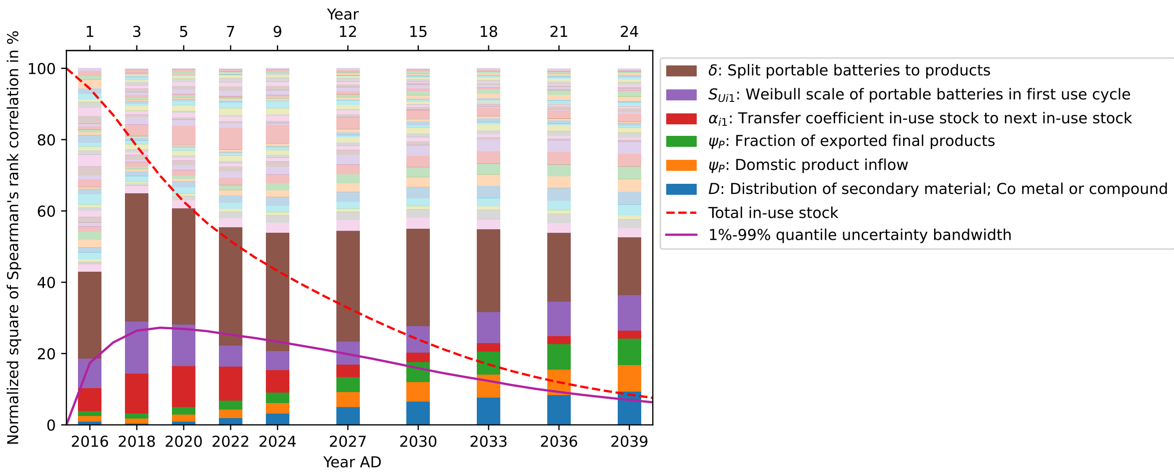

Figure 4.10: Share of uncertainty in total in use-stock by input vectors excluding the three major uncertainty contributor. Transparent contributors are not listed in the legend since their contribution was deemed too small. The dashed red line represents the total in-use stock and the solid purple line represents the 1 % to 99 % quantile uncertainty bandwidth as measure for the uncertainty present at the regarded instances.

The legend presents the six input vectors which hold the largest uncertainty on average. The split of portable battery material to products was already discussed. The Weibull scale for the first use cycle of portable batteries is the next largest contributor. This is in line with the findings above. The parameters defining the lifetime are important. It is also reflected in the third largest parameter in Figure 4.10, the share of products containing portable batteries going directly to a second use cycle. This input is important regarding the total lifetime of a product.

5 Discussion

Driven by future resource scarcity and the implications of raw material extraction this research was conducted to extend and to improve an existing MaTrace model by adding a state of the art representation of a circular strategy (see Table 1.1). Reuse was chosen as the strategy which lead to the following main research question.

How to introduce reuse into a MaTrace model and how to evaluate it?

The first sub-research questions concerns the impact of this venture,:

To what extent is the outcome of the MaTrace model as described by Godoy León et al. (2020) altered, when the reuse of consumer electronics is modelled following the approach of Thiébaud et al. (2017)?

The second sub-research question is concerned with the uncertainties to gain an even better understanding about the model behaviour:

Which input parameters introduce the most uncertainty into the Reuse-MaTrace model and what insights can be derived from analysing uncertainties?

The following will discuss to what extent this research can answer those questions. In order to answer the first part of the main research question, the modelling approach and its limitations will be discussed. The used data, assumptions and uncertainties will be reviewed before diving into the model output and impact answering the first sub-research question. In order to answer the second sub-research question, the outcomes of the Monte Carlo simulations will be interpreted. On this basis the second part of the main research question shall be answered.

The final section of this chapter entails recommendations and suggestions for further research.

5.1. Modeling approach and limitations of the model

The presented Reuse-MaTrace model combines two existing models. The novelty of this work is the application of the two models in interrelation to each other. The MaTrace model by Godoy León et al. (2020) describes the effects of the recycling of cobalt in the EU while the reuse model by Thiébaud et al. (2017) adds another circular strategy to the model.

Although, reuse was considered in previous MaTrace models (Klose & Pauliuk, 2021; Pauliuk et al., 2017; Zhang et al., 2019) this is the first model which follows the approach of Thiébaud et al. (2017) considering individual use, reuse and hibernating times for different products and multiple use cycles. Previous MaTrace implementations modeled reuse in a more simplistic way redirecting end-of-life products back to the in-use stock without considering changes in lifetime.

The two used models are very different in nature. The MaTrace model appears to be very technical on first glance. It relies to a large extend on economic and technical input. The data origin of the reuse model is based on the outcome of social scientific research while the model itself follows a typical MFA approach. Therefore, the newly created model builds an important interface between social science (e.g., lifetimes and reuse), economics (e.g., sales numbers and exports), and natural science/engineering (e.g., recycling efficiencies).

As it was discussed in Section 5.3 the inputs originating from social science research namely the lifetime of products containing portable batteries and the share of products being lost due to non-selective collection determine to a large extend the resource efficiency of cobalt. The model has those numbers as inputs but the underlying concepts and mechanisms are not reflected. Chapter 1 describes that a product can become obsolete to the user for many reasons which determines at least the time of a use-cycle if not the entire lifetime. Furthermore, the knowledge and perception towards waste management determines (alongside with other factors) how well households are separating their waste. Those concepts are not reflected in the model.

This critical property limits the usefulness of the Reuse-MaTrace model for decision and policy makers. The necessary model input regarding those crucial factors can be gathered by conducting interviews and surveys. So, it is possible to model a current state. Furthermore, it is possible to develop desired states by applying scenarios with e.g., longer lifetimes or lower non-selective collection rates. The model can present the current state and what needs to be achieved but not how to do so.

Another limitation of the model is its incompleteness assuming the target is to implement all possible strategies as presented in the 9R-framework (see Table 1.1). The first cluster of suggested strategies "Smarter product use and manufacture" holds strategies which impacts can be reflected via the input data (e.g., R2: Reduce - lowering the inflow of new products). However, the strategies in the second cluster "Extend lifespan of product and its parts" concern the fate of a product at its end of life. Thus, those strategies can be integrated into the Reuse-MaTrace model. Figure 5.1 shows a simplified conceptual integration of those strategies into the model.

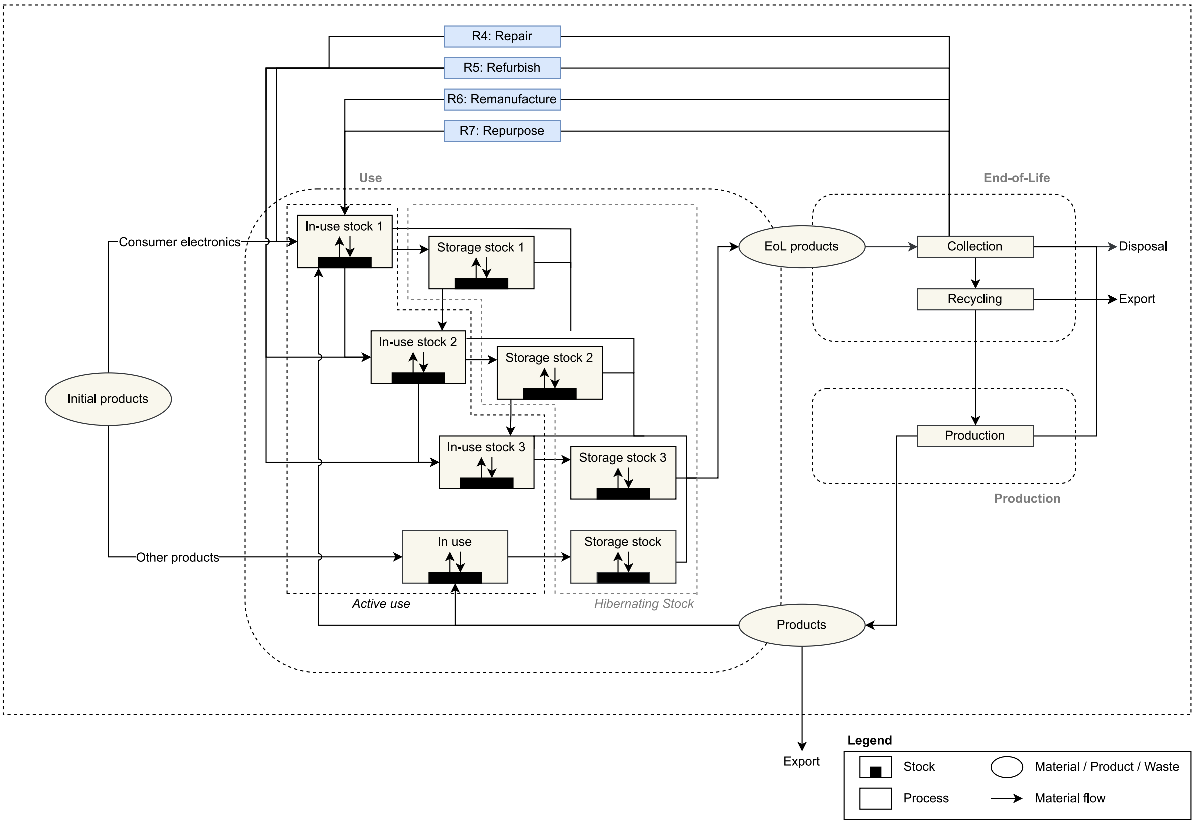

Figure 5.1: Simplified conceptual integration of 9R strategies (in blue) into the Reuse-MaTrace model

Looking at this depiction it must be kept in mind that the representation is highly simplified and that integration of each strategy deserves as much or more thought than the integration of reuse. Considering for example refurbishment, it has to be figure out to which use-cycle the refurbished product can be matched. Is it a as good as new product, or may it become obsolete sooner due to one of the various kinds of obsolescence (see Section 1.1.3)? It might also be that a separate in-use stock for refurbished products has to be introduced since feeding the products back to any use-cycle may not be an adequate modeling choice at all. Those kind of considerations have to be discussed in future research.

The following section treats the used data and its inherent uncertainties since the results of the case study and the Monte Carlos simulation depend to a large extend on this.

5.2. Used data and uncertainties

The data of the model originates from three different main sources. The data for the use phase of non-consumer products, the end of life phase and the production phase are taken from Godoy León et al. (2020) who gathered and assessed their data in their previous publication (Godoy León & Dewulf, 2020). The data for the use phase of portable batteries originates from Glöser-Chahoud et al. (2019)). I extended this data set in order to introduce more diversity in product lifetimes (see Chapter 3).

The data quality and uncertainties were already discussed extensively in Section 2.4.2. As it can be derived from the uncertainty scores (see Appendix B) the bigger share of the received scores are larger than 2 which leads to the conclusion that the data quality is overall low. This has important implications for multiple potential stakeholders as modelers who might have an interest to further develop the model or who get inspired. It is important to recognize that this low availability of high quality data is a source of uncertainty beyond the made assumptions and implications of the model itself. Although one might intuitively think that expanding models might bring more precise results this does not necessarily hold true when the additionally required data is as uncertain. Therefore, it is important to critically assess data availability before taking the decision to apply parts of the model or to extend this model.

The knowledge and consideration of the data quality is equally important for model users who might be in the position to communicate the results or who might base decision on the model output. It has to be understood that the output can only be as good as the model itself in interrelation with the data quality. When the model is applied on another use case it appears to be sensible to execute Monte Carlo simulation as it was done in this research. This helps to gain an understanding about the possible magnitude of the divergence between results and reality.

Although, other interested industrial ecologist may not plan to use the model or its results it is important to realize how hard it is to find valid data to describe societies metabolism. Besides the modeling of material flow, research regarding the accounting and quantification is still urgently needed.

5.3. Impact and model output

Looking at the impact of considering multiple use-cycles, it was found that the total in-use stock increases by 8 % when three use cycles are considered instead of one. Even though, this result is only representative for this specific case study, it shows the clear potential of reuse regarding the in resource efficiency.

The general stock dynamics were described in Section 4.1 and several conclusions can be derived from those and from Figure 4.1. There are four stocks which mainly define the total in-use stock: portable batteries, dissipative uses, hard metals, and super alloys. The case of disspative uses was discussed in Section 4.1. Looking at hard metals and super alloys, it became obvious that those stocks deplete the slowest. The underlying reason for this is most likely their long lifetime. Furthermore, it can be seen that the portable battery stock depletes the quickest, even though reuse is considered. This dynamic has sever consequences regarding the total in-use stock and therefore for the resource efficiency. Portable batteries make up the largest share of the original inflow.

Although, the consideration of reuse changes the magnitude of the total in-use stock significantly in a relevant time frame of the considered period, it does not change the overall stock and flow dynamics. The dynamics as described above are inline with the findings of Godoy León et al. (2020).

But the possibility of reusing products is also a symptom of another threat regarding resource efficiency. Consumers discard functioning products due to various kinds of obsolescence as described in Section 1.1.3. Makov and Fitzpatrick (2021) pointed out, that perceived obsolescence is normally driven by non-technical aspects and consumers tent to underestimate the performance of products they perceive as obsolete.

Since this specific case study treats the reuse of portable batteries, it needs to be considered that portable batteries are components with a rather short lifetime in comparison to other parts of the products. Their expected lifetime lies within three to five years (Beaulieu, 2021). This means that some batteries may have an actual potential to reach their technical end of life while the functional lifetime of batteries also depends on the charging habits of the users.

Another outstanding finding reflected in Figure 4.1 is the distribution of losses and the fact that the largest share of lost material is due to non-selective collection (this finding is as well in line with the findings of Godoy León et al. (2020)). This misplacement of products into the wrong waste collection stream is present for consumer products (portable batteries) but as well for catalysts and hard metals. Hence, the largest loss in the system is not caused by technical limitations but by human error.

The next largest losses are pre-treatment, recycling, and production losses. This is the order in which the processes (pre-treatment, recycling, and production) occur within the system. This circumstance can explain the order of largest losses. By the time the material reaches the production, a large share of it was already lost in the steps before. Therefore the share of production waste is small by default. Therefore, one has to look at the actual efficiencies of the processes since Figure 4.1 might be misleading in that regard. It can be said though, that an increase in recycling and production efficiency can only lead to a relevant gain in overall resource efficiency once less material is lost due to non-selective collection. The overall efficiency of a process chain is calculated via the product of all efficiencies. Hence, all efficiencies have to be high to achieve an overall high efficiency.

Another large share is the accumulated share of exported material. It consist of EOL products, secondary materials, and produced products. The whereabouts of that outflow are not treated by this model.

In summary it can be said, that the consideration of reuse has a significant impact on the total in-use stock. Furthermore, regarding this case study it can be said that further improvements of lifetimes and the recycling performance could be achieved through a change in user behaviour.

5.4. Monte Carlo Simulations

Looking at the outcome of the Monte Carlos simulations regarding the total in-use stock, the main contributor to uncertainty is easily identifiable. Figure 4.8 shows clearly that the split of the initial inflow δ is the input vector which carries the most uncertainty by a large margin. The second most uncertain input vector is the one defining the Weibull scales T for the product categories where products are not reused (all except *portable batteries*). The Weibull scale defines the point in time when 63.2 % of the stock is depleted. Therefore, it determines the survival curve of a product category to a large extent. Considering the article of Miatto et al. (2017) as discussed in Section 1.1.5, it is surprising that Weibull shapes do not contribute much uncertainty in this case study. The shapes of used survival curves are commonly considered to be a source of uncertainty in MFA modelling. The low impact of the shape (in this case) might be due to the variation mechanism used for Weibull shapes. If the initial Weibull shape was larger then 1, the variations considered in the Monte Carlo simulations were limited to values larger then 1. This was done to avoid too large variations in shapes. Hence, this finding may not be generalizable.

Focusing on what can be said based on the results, it became clear by looking at Figure 4.9 that the initial inflow distribution is so important because the lifetimes among the product categories differentiate extremely. The product category with the longest lifetime is super alloys ($T = 17.3$) and the one with the shortest is pet precursors catalyst ($T = 0.57$) (see Appendix A). The Weibull scales were varied by ±50 % which means that the longest lifetime could have never become the smallest and vise versa. Hence, the split of the initial inflow δ contributes more to the variance of the result since this has a larger impact on the survival of the total in-use stock then the variation of the survival curves itself.

Comparing the outcome of the Monte Carlo simulations with the results as presented in Section 4.1 and as discussed in Section 5.3 one might expect to see the largest loss due to non-selective collection reflected. This is not the case. The collection-to-recycling rate σ is not even relevant in Figure 4.10 which displays minor contributors to the uncertainty in the in-use stock. There are two possible explanations for this inconsistency in results. Firstly, its possible that the magnitude in variation of the collection-to-recycling rate σ was too low. Looking at Table B.10 in Appendix B one finds that σ is rated with an uncertainty score of 2 for many product categories including portable batteries (holding the largest share of the initial stock). σ is not varied very strongly due to this low uncertainty. Therefore, it is possible that other inputs had a larger impact on the total in-use stock which is why no correlation was found. Secondly, it could be that there is indeed no strong correlation. As explained in Section 5.3 it might be that a significant share of material is lost in the recycling process once a better waste separation is achieved. Hence, it is possible that a local improvement does not advance the overall performance of the system significantly.

The target of the Monte Carlo simulations was to learn more about the uncertainties of the model itself. The approach taken was only successful to a limited extend since the largest reveled uncertainties are still connected to the initial input data. This insight is not surprising considering the used approach. The inputs were varied based on the estimated uncertainty in the input data. An variation mechanism independent from the data quality might have revealed phenomena closer connected to the model itself instead of the data. Furthermore, the consideration of other distributions to model survival curves may have given interesting insights.

Furthermore, it would have been interesting to see the extension of the MaTrace model reflected in the results. However, it is not necessarily bad that input parameters to the reuse part of the model were not contributing much uncertainty. It could be prove that the extension by the reuse model changes the results significantly (see Section above and Section 4.2.2). Therefore, it can be concluded that the model extension adds detail without increasing the uncertainty significantly.

Another very important learning can be derived from the results of the Monte Carlo simulations: The distribution of the material over the different product categories is more sensitive than the survival curves of these categories. This has implications for different stakeholders. If modelers extend this model they have to be aware that this input needs a lot of attention to determine the shares as accurate as possible. Same holds true for model users applying the model to another context. In both cases it is recommended to execute Monte Carlo simulations because as described, the uncertainties revealed depend to an extend on the input data. Focusing on this specific case study one realizes that an effective way to improve resource efficiency is to decrease the material inflow into product categories with short lifetimes (e.g. pet precursors catalyst or portable batteries).

5.5. Recommendations

On the basis of the created model, the results, and the discussion multiple recommendations for further research can be derived. To begin with, the model behaviour is not sufficiently explored yet although Monte Carlo simulations were conducted. Therefore, I recommend to apply this model on other materials and other geographic regions to test the model with diverse data sets.

Throughout this work, data and data quality played an important role. By scoring the data it became clear that a large share of the inputs are rather uncertain. Therefore, more research and more data collection has to be conducted to obtain high quality data.

Looking at the model itself, there are multiple possibilities to further extend the model. As suggested in Section 5.1, the integration of the 9R framework into the model could be pushed by implementing the strategies repair, refurbish, remanufacturing, or repurpose. A possible starting point to integrate remanufacturing could be the work of Zhang et al. (2021) which integrated the reuse of old vehicle engines in new vehicles into their MaTrace model.

The integration of reuse adds a dimension of consumer behaviour to the model. Although, this work may be a step in the right direction it does not consider consumer behaviour sufficiently. Regarding the results of the case study, a reoccurring finding is the potential influence of consumer behaviour. Consumer behaviour influences the distribution of the initial inflow, lifetimes, hording times, reuse rates, and waste separation - all key aspects regarding resource efficiency. Therefore, more research on how to represent consumer behaviour in MFA models needs to be conducted.

Looking at the overall model output as presented in Figure 4.1, I found that exports make up a large share in the long run. The whereabouts of the exports are admittedly a blind spot of this model. A model solving this problem is MaTrace Global by Pauliuk et al. (2017). Therefore, combining the concepts of Reuse-MaTrace and MaTrace Global might offer insights when investigating the impact of circular strategies on a global scale.

The fact that MaTrace models generally only consider the inflow of one cohort is an obvious weakness. Although, MaTrace models depend on dynamic stock modelling they only consider the inflow of this single year while leaving other parameters as transfer coefficients and efficiencies static. This applies to this thesis as well. As MFA evolved from static to dynamic models, this process has to be repeated for MaTrace models. Therefore, I recommend to create MaTrace models using time series data, both for inflows and other model parameters.

6
Conclusion

The conviction that circular strategies have a positive impact on resource efficiency led to the research objective; integrating a compelling reuse model into a MaTrace model. Reuse has been integrated into MaTrace models before, but as described only in simplistic ways. Therefore, the research question asks: *How to introduce reuse into a MaTrace model and how to evaluate it?*

The first part of this research question was answered methodologically: A state of the art reuse model was found and integrated into the MaTrace model. Consumer goods present in the original MaTrace model are portable batteries. The inflow into this product category was redirected into the reuse model. There the inflow was split into a diverse group of consumer electronics which passed through the reuse model. The outflow, the end of life products, of the reuse model were then fed back into the original MaTrace model which represents the end of life treatment, recycling, and production. The first sub-research question asked about the impact of the consideration of reuse. It was found that the total in-use stock increases by 8 % in the peak when reuse is considered. Hence, it was concluded that the consideration of reuse can have a significant impact on the modeled in-use stock. Beside this, the gross stock dynamics remained intact. The overall findings are in line with the results of Godoy León et al. (2020), the creator of the used MaTrace model.

The second part of the main research question on the evaluation of the model also inspired the second sub-research question. It asked which inputs introduce the most uncertainty into the created Reuse-MaTrace model. On this basis Monte Carlo simulations were conducted in order to gain insights regarding the model behaviour. It was evaluated which model inputs have the largest impact on the total in-use stock, since this was deemed the relevant measure regarding resource efficiency. An assigned input uncertainty score defined how the inputs were varied. The results showed that the by far most influential input parameter is the split of the inflow. This is due to the strongly diverging lifetimes among product categories. This was followed by the lifetimes themselves.

The results of the conducted Monte Carlo simulations gave valuable insights since it identified the most sensitive model inputs. However, the results appear to be strongly connected to the input data and can be hardly generalized to describe the pure model behaviour. A more rigorous randomization mechanism detached from data uncertainty may have served this purpose better.

On the basis of this work multiple ideas for further research came to mind. To start with, this work added only one circular strategy to the MaTrace model. Other circular strategies can be implemented to obtain a more complete representation of a circular economy.

Drawing a parallel of between the evolution of MaTrace models and the development of MFA in recent decades, MaTrace models have to become dynamic. Therefore, I suggest the development of MaTrace models using time series data for inflows and other model parameters.

Lastly, the integration of the reuse model added a dimension of consumer behaviour to MaTrace. The results of the case study revealed that consumer behaviour also influences other parts of the model as the waste treatment process. I recommend to find better ways to consider and represent consumer behaviour in MaTrace models. That way the interface between MFA modelling and social science can grow and strengthen the interdisciplinarity in modelling society's metabolism.

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A

Model input data

A.1. Use phase

Product categories	Initial inflow split ε	Weibull shape β	Weibull scale T
portable batteries	0.412		
mobility batteries	0.012	2.2	10.63150071
hydroprocessing catalysts coke	0.020	2.5	2.894741746
hydroprocessing catalysts poisoning	0.000	2.5	1.505265708
hydroformylation catalysts	0.003	2.5	2.315793397
pet precursors catalysts	0.017	2.5	0.578948349
dissipative uses	0.090	3.5	14.43516632
hard metals	0.230	1.16	8.915234823
magnets	0.006	1.93	13.90502246
other metallic uses	0.002	1.47	14.62806396
superalloys	0.208	1.74	17.28254338

Table A.1: Inputs initial flow split and Weibull parameters for all product categories except for portable batteries

Products	Hoarding rate	Hoarding time (years)
portable batteries	0.520	4
mobility batteries	0.000	0
hydroprocessing catalysts coke	0.000	0
hydroprocessing catalysts poisoning	0.000	0
hydroformylation catalysts	0.000	0
pet precursors catalysts	0.000	0
dissipative uses	0.000	0
hard metals	0.670	1
magnets	0.500	5
other metallic uses	0.500	5
superalloys	1.000	5

Table A.2: Inputs for hibernating stock of all product categories except for portable batteries

Products	Split portable batteries to products δ
smartphones	0.185
mobile phones	0.018
tablets	0.173
laptops	0.350
e-bikes	0.063
power tools	0.041
others	0.170

Table A.3: Inputs split portable batteries to products

Products	Weibull scale T	Weibull shape β	to use α	to storage β
smartphones	2.500	1.700	0.400	0.400
mobile phones	2.000	1.600	0.400	0.500
tablets	4.000	2.000	0.300	0.400
laptops	5.000	2.000	0.200	0.400
e-bikes	4.614	3.000	0.070	0.220
power tools	9.970	1.500	0.050	0.150
others	3.270	2.130	0.210	0.460

Table A.4: Inputs reuse first life-cycle

Products	Weibull scale T	Weibull shape β	to use γ
smartphones	2.500	1.700	0.500
mobile phones	3.500	1.900	0.500
tablets	3.000	1.800	0.300
laptops	3.000	1.800	0.300
e-bikes	2.242	1.700	0.140
power tools	3.362	1.700	0.100
others	2.160	1.170	0.060

Table A.5: Inputs hibernating stock after first use-cycle

Products	Weibull scale T	Weibull shape β	to use α	to storage β
smartphones	2.000	1.600	0.200	0.200
mobile phones	2.000	1.600	0.200	0.200
tablets	2.000	1.600	0.100	0.300
laptops	2.000	1.600	0.100	0.300
e-bikes	4.643	2.500	0.030	0.260
power tools	5.315	1.200	0.020	0.200
others	3.590	2.170	0.080	0.650

Table A.6: Inputs reuse second life-cycle

Products	Weibull scale T	Weibull shape β	to use γ
smartphones	2.000	1.600	0.200
mobile phones	2.000	1.600	0.200
tablets	2.000	1.600	0.300
laptops	2.000	1.600	0.300
e-bikes	1.672	1.590	0.700
power tools	2.229	1.590	0.050
others	3.900	1.460	0.190

Table A.7: Inputs hibernating stock after second use-cycle

Products	Weibull scale T	Weibull shape β	to storage β
smartphones	1.5	1.6	0.3
mobile phones	1.5	1.6	0.3
tablets	2	1.6	0.4
laptops	2	1.6	0.4
e-bikes	2.215464335	1.5	0.29
power tools	2.072726825	1.1	0.3
others	3.59	2.17	0.7

Table A.8: Inputs reuse third life-cycle

Products	Weibull scale T	Weibull shape β
smartphones	2.000	1.600
mobile phones	2.000	1.600
tablets	1.000	1.500
laptops	1.000	1.500
e-bikes	1.672	1.590
power tools	2.229	1.590
others	3.900	1.460

Table A.9: Inputs hibernating stock after third use-cycle

A.2. End-of-life phase

Product categories	Fraction of collected EOL products exported ψ_{EOL}	Collection to recycling rate σ	Pre-treatment efficiency λ_{PT}
portable batteries	0.200	0.640	0.950
mobility batteries	0.000	1.000	0.850
hydroprocessing catalysts coke	0.000	1.000	0.850
hydroprocessing catalysts poisoning	0.000	0.000	0.000
hydroformylation catalysts	0.000	0.900	0.850
pet precursors catalysts	0.000	0.500	0.850
dissipative uses	0.000	0.000	0.000
hard metals	0.000	0.470	0.770
magnets	0.000	0.990	0.650
other metallic uses	0.000	0.840	0.650
superalloys	0.300	0.810	0.650

Table A.10: Inputs collection and pre-treatment

Product categories	Chemical	Zn	Downcycling
portable batteries	1.000	0.000	0.000
mobility batteries	1.000	0.000	0.000
hydroprocessing catalysts coke	0.500	0.000	0.500
hydroprocessing catalysts poisoning	0.000	0.000	1.000
hydroformylation catalysts	1.000	0.000	0.000
pet precursors catalysts	0.000	0.000	1.000
dissipative uses	0.000	0.000	0.000
hard metals	0.630	0.370	0.000
magnets	0.000	0.000	1.000
other metallic uses	0.000	0.000	1.000
superalloys	0.610	0.000	0.390
Recycling efficiency	0.897	0.950	

Table A.11: Inputs distribution to recycling processes B and recycling efficiency

Product categories	Co metal or compound	W-Co powder
portable batteries	0.000	0.000
mobility batteries	0.021	0.000
hydroprocessing catalysts coke	0.014	0.000
hydroprocessing catalysts poisoning	0.014	0.000
hydroformylation catalysts	0.005	0.000
pet precursors catalysts	0.024	0.000
dissipative uses	0.167	0.000
hard metals	0.313	1.000
magnets	0.017	0.000
other metallic uses	0.003	0.000
superalloys	0.423	0.000
Fraction of exported secondary material $\psi_{R}	0.133	0.000

Table A.12: Inputs distribution of secondary material and fraction of exported secondary material

A.3. Production

Product categories	Processing yield λ_P	Manufacturing yield λ_M	Processing scrap recovery ξ_P	Manufacturing scrap recovery ξ_M	Processing downcycled scrap ω_P	Manufacturing downcycled scrap ω_M	Fraction of exported final products ψ_P
portable batteries	0.000	0.000	0.000	0.000	0.000	0.000	0.000
mobility batteries	0.850	1.000	1.000	1.000	0.000	0.000	0.000
hydroprocessing catalysts coke	0.970	0.960	1.000	1.000	0.000	0.000	0.000
hydroprocessing catalysts poisoning	0.970	0.960	1.000	1.000	0.000	0.000	0.000
hydroformylation catalysts	0.970	0.010	1.000	1.000	0.000	0.000	0.000
pet precursors catalysts	0.970	0.970	1.000	1.000	0.000	0.000	0.000
dissipative uses	0.970	0.950	1.000	1.000	0.000	0.000	0.380
hard metals	0.980	1.000	1.000	1.000	0.000	0.000	0.460
magnets	0.940	0.960	0.000	0.000	0.500	0.000	0.620
other metallic uses	0.750	0.790	0.680	0.690	0.290	0.450	0.440
superalloys	0.710	0.470	0.950	0.470	0.560	0.890	0.610

Table A.13: Inputs production

B

Uncertainty scoring of Input uncertainty scoring

Scores marked with a star (*) base on the evaluation of assessment of Godoy León and Dewulf (2020) as follows:

- Uncertainty score 1: "Very high data quality"
- Uncertainty score 2: "High data quality"
- Uncertainty score 3: "Low data quality"
- Uncertainty score 4: "No data reported"

All other scores base on the perception of the author. The reasoning is explained in Section 2.4.2 and in the captions of the tables.

B.1. Use phase

Product categories	Initial inflow split ε	Weibull shape β	Weibull scale T
portable batteries	2*	0*	0*
mobility batteries	2*	1*	4*
hydroprocessing catalysts coke	2*	2*	4*
hydroprocessing catalysts poisoning	2*	2*	4*
hydroformylation catalysts	2*	2*	4*
pet precursors catalysts	2*	1*	4*
dissipative uses	2*	2*	3*
hard metals	2*	1*	2*
magnets	2*	1*	2*
other metallic uses	2*	1*	2*
superalloys	2*	1*	2*

Table B.1: Input uncertainty scoring initial flow split and Weibull parameters for all product categories except for portable batteries

Products	Hoarding rate	Hoarding time (years)
portable batteries	0	0
mobility batteries	2*	2*
hydroprocessing catalysts coke	4*	4*
hydroprocessing catalysts poisoning	4*	4*
hydroformylation catalysts	4*	4*
pet precursors catalysts	4*	4*
dissipative uses	2*	2*
hard metals	3*	2*
magnets	4*	4*
other metallic uses	4*	4*
superalloys	3*	3*

Table B.2: Input uncertainty scoring for hibernating stock of all product categories except for portable batteries

Products	Split portable batteries to products δ
smartphones	4
mobile phones	4
tablets	4
laptops	4
e-bikes	4
power tools	4
others	4

Table B.3: Input uncertainty scoring split portable batteries to products. The uncertainty is high. The split bases on a single source and was adapted to fit the considered products. The split of portable batteries to products bases on one non-scientific source and is therefore scored with 4.

Products	Weibull scale T	Weibull shape β	to use α	to storage β
smartphones	2 (a)	1 (a)	3 (b)	3 (b)
mobile phones	2 (a)	1 (a)	3 (b)	3 (b)
tablets	2 (a)	1 (a)	3 (b)	3 (b)
laptops	2 (a)	1 (a)	3 (b)	3 (b)
e-bikes	4	2	4	4
power tools	4	2	4	4
others	4	2	4	4

Table B.4: Input uncertainty scoring reuse first life-cycle. (a) the data bases on empirical studies, (b) the data bases on the literature review and assumptions of Glöser-Chahoud et al. (2019), and the rest of the data bases on own assumptions.

Products	Weibull scale T	Weibull shape β	to use γ
smartphones	2 (a)	1 (a)	3 (b)
mobile phones	2 (a)	1 (a)	3 (b)
tablets	2 (a)	1 (a)	3 (b)
laptops	2 (a)	1 (a)	3 (b)
e-bikes	4	2	4
power tools	4	2	4
others	4	2	4

Table B.5: Input uncertainty scoring hibernating stock after first use-cycle. (a) the data bases on empirical studies, (b) the data bases on the literature review and assumptions of Glöser-Chahoud et al. (2019), and the rest of the data bases on own assumptions.

Products	Weibull scale T	Weibull shape β	to use α	to storage β
smartphones	3	2	4	4
mobile phones	3	2	4	4
tablets	3	2	4	4
laptops	3	2	4	4
e-bikes	5	2	5	5
power tools	5	2	5	5
others	5	2	5	5

Table B.6: Input uncertainty scoring reuse second life-cycle. The data sources are the same as in Table B.4. It is assumed that the certainty of the data gets worse in the second use cycle (also see Section 2.4.2).

Products	Weibull scale T	Weibull shape β	to use γ
smartphones	3	2	4
mobile phones	3	2	4
tablets	3	2	4
laptops	3	2	4
e-bikes	5	2	5
power tools	5	2	5
others	5	2	5

Table B.7: Input uncertainty scoring hibernating stock after second use-cycle. The data sources are the same as in Table B.5. It is assumed that the certainty of the data gets worse in the second use cycle (also see Section 2.4.2).

Products	Weibull scale T	Weibull shape β	to storage β
smartphones	5	2	5
mobile phones	5	2	5
tablets	5	2	5
laptops	5	2	5
e-bikes	5	2	5
power tools	5	2	5
others	5	2	5

Table B.8: Input uncertainty scoring reuse third life-cycle. All inputs have the worst score possible. It is assumed that the base of knowledge of the previous whereabouts of the product is very low.

Products	Weibull scale T	Weibull shape β
smartphones	5	2
mobile phones	5	2
tablets	5	2
laptops	5	2
e-bikes	5	2
power tools	5	2
others	5	2

Table B.9: Input uncertainty scoring hibernating stock after third use-cycle. It is assumed that the base of knowledge of the previous whereabouts of the product is very low.

B.2. End-of-life phase

Product categories	Fraction of collected EOL products exported ψ_{EOL}	Collection to recycling rate σ	Pre-treatment efficiency λ_{PT}
portable batteries	4*	2*	2*
mobility batteries	4*	4*	4*
hydroprocessing catalysts coke	4*	4*	4*
hydroprocessing catalysts poisoning	4*	4*	4*
hydroformylation catalysts	4*	4*	4*
pet precursors catalysts	4*	4*	4*
dissipative uses	4*	0*	0*
hard metals	4*	3*	1*
magnets	4*	2*	3*
other metallic uses	4*	2*	4*
superalloys	4*	2*	4*

Table B.10: Input uncertainty scoring collection and pre-treatment

Product categories	Chemical	Zn	Downcycling
portable batteries	4*	4*	4*
mobility batteries	4*	4*	4*
hydroprocessing catalysts coke	3*	3*	3*
hydroprocessing catalysts poisoning	3*	3*	3*
hydroformylation catalysts	4*	4*	4*
pet precursors catalysts	4*	4*	4*
dissipative uses	0*	0*	0*
hard metals	3*	3*	3*
magnets	0*	0*	0*
other metallic uses	0*	0*	0*
superalloys	2*	2*	2*
Recycling efficiency	2*	2*	0*

Table B.11: Input uncertainty scoring distribution to recycling processes B and recycling efficiency

Product categories	Co metal or compound	W-Co powder
portable batteries	0*	0*
mobility batteries	4*	4*
hydroprocessing catalysts coke	4*	4*
hydroprocessing catalysts poisoning	4*	4*
hydroformylation catalysts	4*	4*
pet precursors catalysts	4*	4*
dissipative uses	4*	4*
hard metals	4*	4*
magnets	4*	4*
other metallic uses	4*	4*
superalloys	4*	4*
Fraction of exported secondary material $\psi_{R}	3*	4*

Table B.12: Input uncertainty scoring distribution of secondary material and fraction of exported secondary material

B.3. Production

Product categories	Processing yield λ_P	Manufacturing yield λ_M	Processing scrap recovery ξ_P	Manufacturing scrap recovery ξ_M	Processing downcycled scrap ω_P	Manufacturing downcycled scrap ω_M	Fraction of exported final products ψ_P
portable batteries	0*	0*	0*	0*	0*	0*	0*
mobility batteries	2*	4*	4*	4*	4*	4*	4*
hydroprocessing catalysts coke	3*	3*	4*	4*	4*	4	4*
hydroprocessing catalysts poisoning	3*	3*	4*	4*	4*	4*	4*
hydroformylation catalysts	3*	4*	4*	4*	4*	0*	4*
pet precursors catalysts	3*	4*	4*	4*	4*	4*	4*
dissipative uses	3*	3*	4*	3*	4*	3*	4*
hard metals	2*	2*	4*	2*	4*	2*	4*
magnets	2*	2*	4*	2*	2*	2*	4*
other metallic uses	3*	3*	3*	3*	3*	3*	4*
superalloys	2*	2*	3*	2*	3*	2*	4*

Table B.13: Input uncertainty scoring production

C
Monte Carlo simulations input distributions

This appendix entails three graphs showing how those selected inputs were varied for the Monte Carlo simulations.

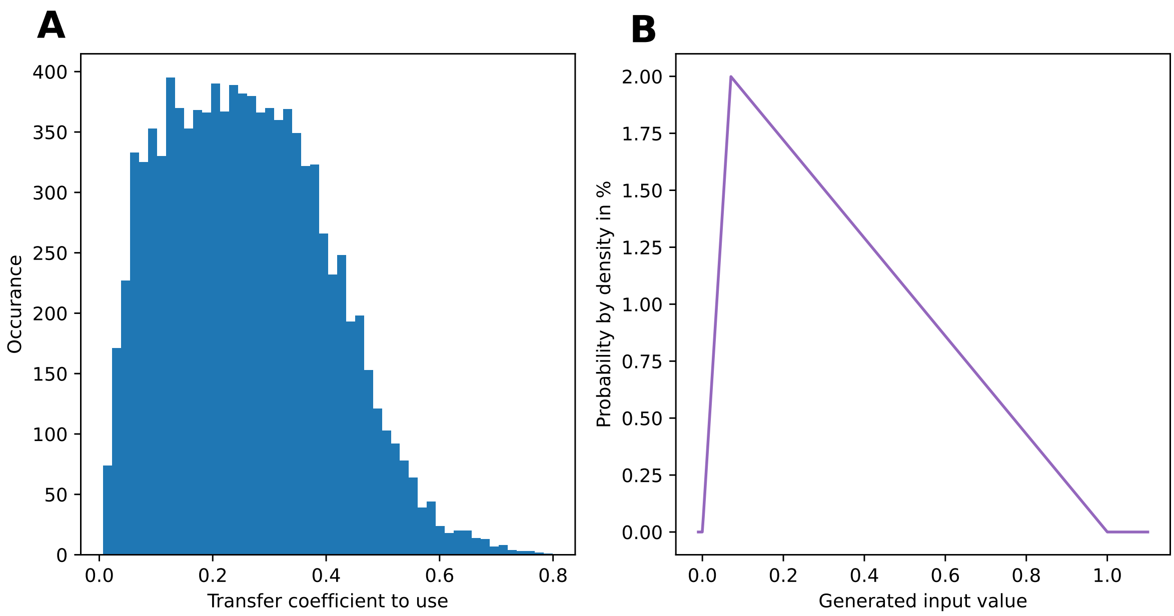


Figure C.1: Histogram (a) and defined distribution (b) of the transfer coefficient to use in the first use cycle for e-bikes. The actual input value is 0.07 and the assigned uncertainty score is 4. As it can be seen, the histogram does not really match the defined distribution. This is because the created value was normalized with other transfer coefficients to ensure that they sum up to 1. This is done to insure mass conservation.

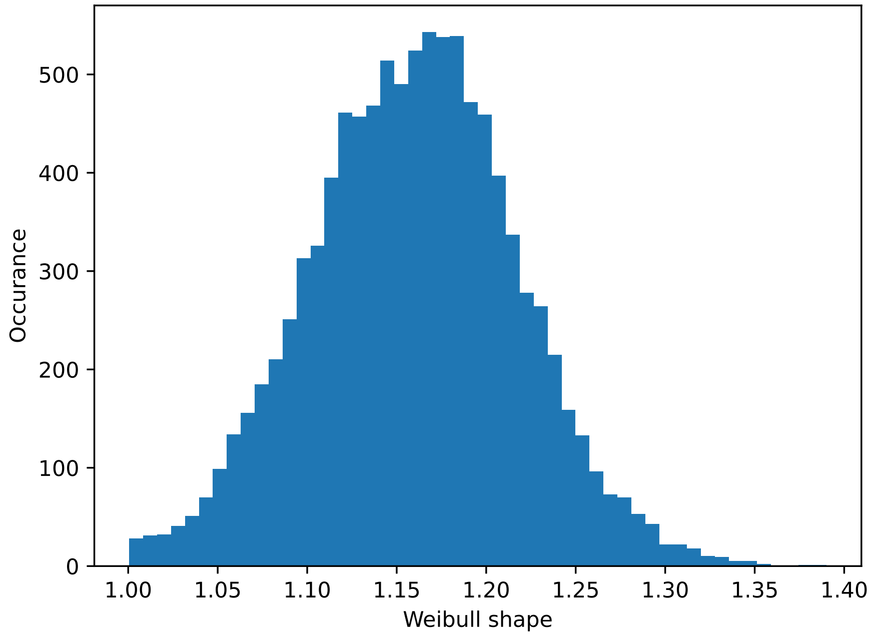


Figure C.2: Histogram of the Weibull shape for the in-use time of hard metals. The actual input value is 1.16 and the uncertainty score is 1. As it can be seen, there are no values below 1 (for explanation see Section 2.4.2).

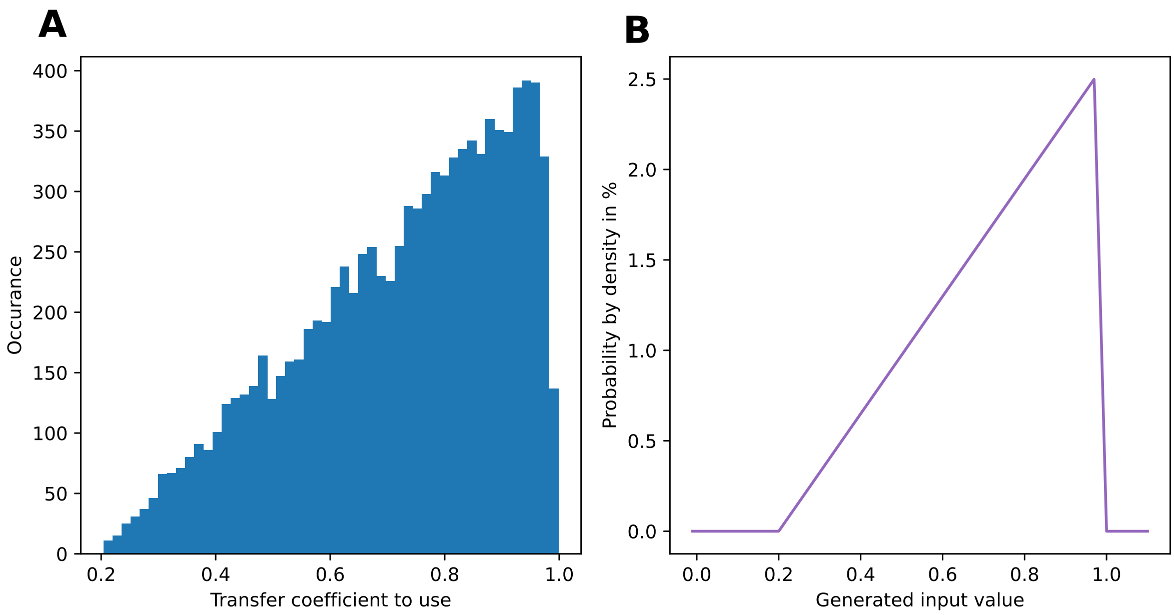


Figure C.3: Histogram (a) and defined distribution (b) of the efficiency of the production process for dissipative uses. The actual input value is 0.97 and the assigned uncertainty score is 3. As it can be seen, the histogram follows the defined distribution (in contrast to Figure C.1). This is because efficiencies do not have to be normalized with any other values.

D

Model application manual and description of digital appendix

The model application manual can be found from the next page onwards. It consist out of a Jupyter Notebook explaining how to use the model and how to use the provided scripts to execute Monte Carlo simulations. The notebook is also provided as html file which can be opened in the browser. The names of those files are:

- model_application_manual.ipynb
- model_application_manual.html

The digital appendix consists of multiple files and folders. The model itself is defined by the following files:

- base_matrace_model.py
- base_reuse_model.py
- combined_reuse_matrace_model.py

The following files are needed to execute and evaluate the Monte Carlo simulations:

- functions.py
- monte_carlo_simulations.py
- monte_carlo_evaluation.py
- monte_carlo_uncertainty.py

Furthermore, there is a notebook (also as html) with all graphs used throughout this thesis:

- used_graphs.ipynb
- used_graphs.html

There are three folders in the digital appendix. The folder "data_cobalt_case_study" holds the data used for the case study as well as the results of the Monte Carlo simulations. The folder "data_model" holds exemplary data used in the model manual. The folder "monte_carlo_results" is necessary in order to execute the Jupyter Notebook containing the model application manual.

Model application manual

This notebook describes how to apply the model on different data as presented in the thesis. It will be explained:

- How to create a data set readable by the model
- How to execute the model itself
- And how to conduct Monte Carlo Simulations with the provided code

How to create a readable data set

Creation of a readable data set

The created model requires an excel file in a specific format. A function was created to create a plain excel file in the right format. The function requires a list entailing the product categories which are treated by the model, a string naming the product category which flows into the reuse part of the model, a list indication the products treated in the reuse part of the model, and the number of considered use cycles in the reuse part. Furthermore, a file name has to be provided. The created file will appear in the "data_model" folder.

In [ ]:

```
from functions import input_file_creator

input_file_creator(
    product_categories=['electronics', 'cars', 'industrial applications'],
    category_for_reuse='electronics', products=['shaver', 'phone', 'TV'],
    considered_use_cycles=2, file_name = 'example_file_creator')
```

All sheets of the file are empty and to be filled by the user.

In [ ]:

```
import pandas as pd
pd.read_excel('data_model/example_file_creator.xlsx')
```

Out[ ]:

	Product categories	share
0	electronics	NaN
1	cars	NaN
2	industrial applications	NaN

In [ ]:

```
import os
os.remove('data_model/example_file_creator.xlsx')
```

To showcase how to input data, an example file will be considered.

Things to consider populating the data frame

A few sheets are presented as examples. In general, common-sense mistakes need to be avoided.

Ensuring mass conservation when splitting the material flow

The following output shows the first sheet, the split of the initial inflow.

In [ ]:
```
pd.read_excel('data_model/data_example.xlsx', sheet_name='MaTrace_initial_inflow')
```

Out[ ]:

	Product categories	share
0	electronics	0.412
1	mobility batteries	0.012
2	hydroprocessing catalysts coke	0.020
3	hydroprocessing catalysts poisoning	0.000
4	hydroformylation catalysts	0.003
5	pet precursors catalysts	0.017
6	dissipative uses	0.090
7	hard metals	0.230
8	magnets	0.006
9	other metallic uses	0.210

The sum of this column has to equal 1.

In [ ]:
```
pd.read_excel('data_model/data_example.xlsx',
    sheet_name='MaTrace_initial_inflow')['share'].sum(axis = 0)
```

Out[ ]:
```
1.0
```

The same holds true for the sheet "Reuse_inflow_split".

In [ ]:
```
pd.read_excel('data_model/data_example.xlsx', sheet_name='MaTrace_initial_inflow')
```

Out[ ]:

	Product categories	share
0	electronics	0.412
1	mobility batteries	0.012
2	hydroprocessing catalysts coke	0.020
3	hydroprocessing catalysts poisoning	0.000
4	hydroformylation catalysts	0.003
5	pet precursors catalysts	0.017
6	dissipative uses	0.090
7	hard metals	0.230
8	magnets	0.006
9	other metallic uses	0.210

And as well for the sheet "MaTrace_D_secondary_material". In this case, the last two rows need to be excluded since the indicate the export and to production rate.

In [ ]:
```python
pd.read_excel('data_model/data_example.xlsx',
    sheet_name='MaTrace_D_secondary_material')
```

Out[ ]:

	Product categories	Co metal or compound	W-Co powder
0	electronics	0.0000	0
1	mobility batteries	0.0210	0
2	hydroprocessing catalysts coke	0.0135	0
3	hydroprocessing catalysts poisoning	0.0135	0
4	hydroformylation catalysts	0.0050	0
5	pet precursors catalysts	0.0240	0
6	dissipative uses	0.1670	0
7	hard metals	0.3130	1
8	magnets	0.0170	0
9	other metallic uses	0.4260	0
10	export rate	0.1330	0
11	to production rate	0.8670	1

In [ ]:
```python
print(pd.read_excel('data_model/data_example.xlsx',
    sheet_name='MaTrace_D_secondary_material').iloc[:-2, :])
print()
print('Sum of columns without export rate and to production rate:')
print(pd.read_excel('data_model/data_example.xlsx',
    sheet_name='MaTrace_D_secondary_material').iloc[:-2, :].sum(axis=0))
```

```
                    Product categories  Co metal or compound  W-Co powder
0                          electronics                0.0000            0
1                   mobility batteries                0.0210            0
2       hydroprocessing catalysts coke                0.0135            0
3  hydroprocessing catalysts poisoning                0.0135            0
4           hydroformylation catalysts                0.0050            0
5             pet precursors catalysts                0.0240            0
6                     dissipative uses                0.1670            0
7                          hard metals                0.3130            1
8                              magnets                0.0170            0
9                  other metallic uses                0.4260            0

Sum of columns without export rate and to production rate:
Product categories      electronicsmobility batterieshydroprocessing c...
Co metal or compound                                                  1.0
W-Co powder                                                             1
dtype: object
```

Furthermore, some transfer coefficients must sum up to 1. In the model one transfer coefficient is sufficient to define a flow which splits into two. However, for the Monte Carlo simulations both are needed.

The following cell shows the example of the sheet "MaTrace_end_of_life":

In [ ]:
```python
pd.read_excel('data_model/data_example.xlsx', sheet_name='MaTrace_end_of_life')
```

Out[ ]:

	Product categories	fraction export eol products	fraction collected eol products	collection to recycling rate	postconsumer disposal rate	pre-treatment efficiency
0	electronics	0.2	0.8	0.64	0.36	0.95
1	mobility batteries	0.0	1.0	1.00	0.00	0.85
2	hydroprocessing catalysts coke	0.0	1.0	1.00	0.00	0.85
3	hydroprocessing catalysts poisoning	0.0	1.0	0.00	1.00	0.00
4	hydroformylation catalysts	0.0	1.0	0.90	0.10	0.85
5	pet precursors catalysts	0.0	1.0	0.50	0.50	0.85
6	dissipative uses	0.0	1.0	0.00	1.00	0.00
7	hard metals	0.0	1.0	0.47	0.53	0.77
8	magnets	0.0	1.0	0.99	0.01	0.65
9	other metallic uses	0.0	1.0	0.84	0.16	0.65

The column "fraction export eol products" and "fraction collected eol products" as well as the columns "collection to recycling rate" and "postconsumer disposal" have to sum up to 1 for every product category.

Please also consult the system diagram or the excel file data_example.xlsx to find the respective transfer coefficients.

Defining survival curves

The sheet "MaTrace_in_use_stock" show examples on how to define survival curves in the model implementation:

In [ ]:

```
pd.read_excel('data_model/data_example.xlsx', sheet_name='MaTrace_in_use_stock')
```

Out[ ]:

	Product categories	distribution	location	scale	shape
0	electronics	normal	1	4.051716	2.09
1	mobility batteries	weibull	0	10.631501	2.20
2	hydroprocessing catalysts coke	gamma	0	2.894742	2.50
3	hydroprocessing catalysts poisoning	defined_distribution_example_dist	0	0.000000	0.00
4	hydroformylation catalysts	lognormal	1	2.315793	2.50
5	pet precursors catalysts	normal	0	0.578948	2.50
6	dissipative uses	weibull	0	14.435166	3.50
7	hard metals	gamma	0	8.915235	1.16
8	magnets	gompertz	2	13.905022	1.93

	Product categories	distribution	location	scale	shape
9	other metallic uses	lognormal	0	14.628064	1.47

One can select a distribution via the column "distribution". The normal, lognormal, weibull, gamma, and gompertz distribution are preimplemented. The location, scale and shape factors can be set via the corresponding columns. It is also possible to define own distributions.

An example for this is the distribution for the product category "hydroprocessing catalysts poisoning". The string says "defined_distribution_example_dist". This works in the following way. A distribution is defined in the file "defined_distributions.xlsx" (see next cell).

In [ ]:

```
pd.read_excel('data_model/defined_distributions.xlsx').iloc[:10]
```

Out[ ]:

	example_dist	example_dist_2
0	1.00	1.00
1	0.60	0.70
2	0.55	0.55
3	0.50	0.50
4	0.45	0.45
5	0.40	0.40
6	0.35	0.35
7	0.30	0.30
8	0.25	0.20
9	0.20	0.20

The file holds survival curves defined by the user. Only the first 10 lines are shown. It is important that the distribution is defined for a sufficient number of years, meaning at least the number of considered years.

To use this distribution in the model, one has to fill the column "distribution" with "defined_distribution_column_name". Hence, when the entry in the column "distribution" says "defined_distribution_example_dist", the defined distribution "example_dist" will be used for this product category. If it says "defined_distribution_exmaple_dist_2" the distribution "example_dist_2" will be used for the product category.

How to execute the model iteself

The first step to execute the model is to load the required data. The model receives a dictionary as input which contains the sheets of the mentioned excel file as pandas data frames. The following code cell creates this dictionary.

In [ ]:

```
file_path = 'data_model/data_example.xlsx'

data_sheets = pd.ExcelFile(file_path).sheet_names
```

```python
data_dic = {}

for data_sheet in data_sheets:

    try:
        data_dic[data_sheet] = pd.read_excel(file_path,
            sheet_name=data_sheet).set_index('Product categories')
    except:
        data_dic[data_sheet] = pd.read_excel(file_path,
            sheet_name=data_sheet).set_index('Products')
```

Furthermore, the number of years and the start year have to be defined. A pandas dataframe containing the "defined_distributions.xlsx" file has to be passed as well.

In [ ]:

```python
number_of_years = 25
start_year = 2022
defined_distributions_pd = pd.read_excel('data_model/defined_distributions.xlsx')
```

Optionally, one can decide to print the state to have an indication whether the model is stuck or how long it will still run. One can also define whether the simplified model output shall differentiate between use cycles. Lastly, one can select the number of considered use cycles (default is 3).

The following code shows the execution of the model:

In [ ]:

```python
from combined_reuse_matrace_model import evaluate_cohort_combined_model

matrace_data_dic, reuse_data_dic, graph_data_pd = \
    evaluate_cohort_combined_model(data_dic=data_dic,
        n_years=number_of_years, start_year=start_year,
        defined_distributions_pd= defined_distributions_pd,
        print_state=True, separate_reuse_graph=True, considered_use_cycles=3)
```

```
Year 1 of 25
Year 2 of 25
Year 3 of 25
Year 4 of 25
Year 5 of 25
Year 6 of 25
Year 7 of 25
Year 8 of 25
Year 9 of 25
Year 10 of 25
Year 11 of 25
Year 12 of 25
Year 13 of 25
Year 14 of 25
Year 15 of 25
Year 16 of 25
Year 17 of 25
Year 18 of 25
Year 19 of 25
Year 20 of 25
Year 21 of 25
Year 22 of 25
Year 23 of 25
Year 24 of 25
Year 25 of 25
```

The returned dictionaries "matrace_data_dic" and "reuse_data_dic" are structured in the same way. The first key takes a string containing the considered year. The second key takes a string indicating a stock or a flow in the year. This will then return a pandas containing the values over product categories or products.

The following code cell shows the second keys of "matrace_data_dic".

In [ ]:
```
matrace_data_dic['0'].keys()
```

Out[ ]:
```
Index(['U.A use stock', 'U.2 use outflow', 'U.3 hoarding inflow',
       'U.4 no hoarding flow', 'U.B hoarding stock', 'U.5 hoarding outflow',
       'U.6 eol products', 'E.2 exported eol products',
       'E.1 to waste treatment', 'E.3 to pretreatment',
       'E.4 E.5 non-selective collection', 'E.6 to recycling',
       'E.7 pretreatment waste', 'E.12 downcycling', 'recycled w-co powder',
       'co metal compound', 'E.8 recycling waste',
       'E.11 exported recycled materials', 'P.1 total recycled products',
       'P.8 export recycled products', 'U.1 product inflow',
       'P.7 processing waste', 'P.5p downcycled scrap', 'P.4p disposed scrap',
       'P.2 manufacturing waste', 'P.5m downcycled scrap',
       'P.4m disposed scrap', 'P.4 disposed scrap', 'P.5 downcycled scrap'],
      dtype='object')
```

And the following code cell shows the second keys of "reuse_data_dic".

In [ ]:
```
reuse_data_dic['0'].keys()
```

Out[ ]:
```
Index(['total_use_stock', 'total_hoarding_stock', 'to_disposal_flow',
       'use_stock_1', 'storage_stock_1', 'use_1_to_storage_1_flow',
       'use_1_to_disposal_flow', 'storage_1_to_disposal_flow',
       'use_1_to_use_2_flow', 'storage_1_to_use_2_flow', 'use_stock_2',
       'storage_stock_2', 'use_2_to_storage_2_flow', 'use_2_to_disposal_flow',
       'storage_2_to_disposal_flow', 'use_2_to_use_3_flow',
       'storage_2_to_use_3_flow', 'use_stock_3', 'storage_stock_3',
       'use_3_to_storage_3_flow', 'use_3_to_disposal_flow',
       'storage_3_to_disposal_flow'],
      dtype='object')
```

The following code cell shows the content.

In [ ]:
```
reuse_data_dic['0']['total_use_stock']
```

Out[ ]:
```
Products
computer       0.026567
phone          0.045320
fan            0.082400
dish washer    0.185400
e-bikes        0.024720
power tools    0.019502
Name: total_use_stock, dtype: float64
```

In [ ]:
```
matrace_data_dic['0']['U.A use stock']
```

Out[ ]:
```
Products
electronics                               0.38391
mobility batteries                          0.012
hydroprocessing catalysts coke               0.02
hydroprocessing catalysts poisoning           0.0
hydroformylation catalysts                  0.003
pet precursors catalysts                   0.0085
```

```
dissipative uses                          0.09
hard metals                               0.23
magnets                                  0.006
other metallic uses                       0.21
Name: U.A use stock, dtype: object
```

The retuned pandas dataframe "graph_data_pd" contains the stocks and the accumulated outflows.

In [ ]:

```
graph_data_pd
```

Out[ ]:

Year	Electronics 1st use	Electronics 2nd use	Electronics 3rd use	Mobility batteries	Hydroprocessing catalysts coke	Hydroprocessing catalysts poisoning	Hydroform c
2022	0.377540	0.005548	0.000821	0.012176	0.020113	0.000113	0
2023	0.281169	0.017890	0.001593	0.012589	0.020090	0.000421	0
2024	0.199773	0.026279	0.002235	0.012901	0.019297	0.000728	0
2025	0.142881	0.031148	0.002443	0.012958	0.017849	0.000909	0
2026	0.106036	0.032665	0.002545	0.012749	0.016026	0.001010	0
2027	0.083086	0.031205	0.002917	0.012286	0.014056	0.001063	0
2028	0.068224	0.028201	0.003453	0.011605	0.012104	0.001080	0
2029	0.057489	0.024919	0.003829	0.010758	0.010275	0.001073	0
2030	0.047519	0.021968	0.003884	0.009806	0.008634	0.001056	0
2031	0.041138	0.019131	0.003691	0.008783	0.007190	0.001019	0
2032	0.034343	0.016645	0.003386	0.007755	0.005957	0.000974	0
2033	0.028269	0.014450	0.003054	0.006757	0.004920	0.000924	0
2034	0.022851	0.012621	0.002727	0.005817	0.004056	0.000861	0
2035	0.018026	0.011123	0.002423	0.004960	0.003344	0.000788	0
2036	0.014967	0.009819	0.002153	0.004191	0.002755	0.000703	0
2037	0.012373	0.008728	0.001925	0.003523	0.002274	0.000615	0
2038	0.010187	0.007783	0.001740	0.002954	0.001882	0.000538	0
2039	0.008353	0.006950	0.001594	0.002477	0.001563	0.000472	0
2040	0.006823	0.006196	0.001475	0.002081	0.001302	0.000416	0
2041	0.005552	0.005507	0.001374	0.001758	0.001089	0.000368	0
2042	0.004501	0.004883	0.001281	0.001493	0.000916	0.000327	0
2043	0.003637	0.004319	0.001191	0.001278	0.000773	0.000291	0
2044	0.002928	0.003814	0.001101	0.001101	0.000656	0.000258	0
2045	0.002350	0.003365	0.001011	0.000955	0.000559	0.000230	0
2046	0.001880	0.002968	0.000923	0.000834	0.000479	0.000204	0

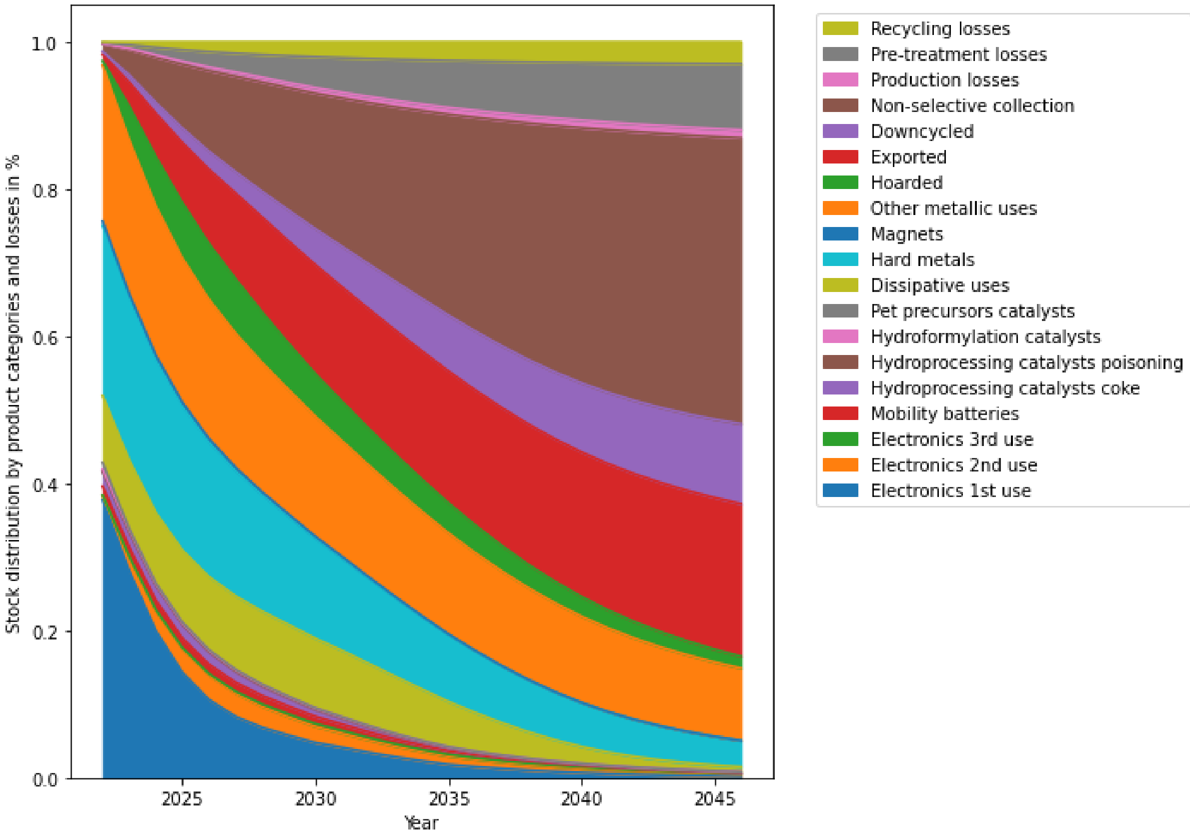
It is easily possible to create a stacked area chart out of it.

In [ ]:
```
import matplotlib.pyplot as plt

plt.rcParams["figure.figsize"] = [10, 7]
graph_data_pd.plot.area()

plt.legend(reversed(plt.legend().legendHandles), reversed(
    graph_data_pd.columns), bbox_to_anchor=(1.05, 1))

plt.ylabel('Stock distribution by product categories and losses in %')
plt.tight_layout()
plt.show()
```



How to conduct Monte Carlo simulations with the provided code

The code to conduct Monte Carlo simulations consists of three files which need to be executed one after another:

- monte_carlo_simulations.py
- monte_carlo_evaluation.py
- monte_carlo_uncertainty.py

In the following it will be discussed what each file does and how to use it. To do so, files and the data used in the cobalt case study will be used. Each of the files has the variable "proof_of_concept" in the very top. If this is "True", an exemplary Monte Carlo simulation and evaluation considering 10 runs will be conducted. If it is set to "False" the results as presented in the thesis will be reproduced.

In [ ]:
```
# The folder holding the results of the following demonstration
# needs to be deleted in order to be created and populated.
# This is a necessary step but not relevant in the context of
# the explenation.
import shutil
try:
    shutil.rmtree('monte_carlo_results/proof_of_concept/')
except:
    print('Dictionary does not excist.')
```

Executing "monte_carlo_simulations.py"

At the start of the file, the user can adjust the settings. Those are the number of runs ("n_runs"), the number of the considered years ("n_years"), the start year ("start_year"), and the number of the considered use cycles ("considered_use_cycles").

Then, the data to be loaded needs to be specified. Firstly, the file entailing the survival curves designed by the user has to be loaded (see above). Secondly, the path to the input data (format as described above) has to be specified. Lastly, the excel file containing the uncertainty rating has to be set.

This file must entail the same sheet names as the input file. Instead of the data, the colums must hold the uncertainty score (0 to 5, as explained in the main body of the thesis).

If an input shall not be varied, the column can be either deleted from the file holding the uncertainty scores, or all values can be set to 0. Only numerical inputs can be considered.

The following cell shows one sheet of the excel holding the input data. The next one shows the uncertainty ratings of those inputs.

In [ ]:
```
pd.read_excel('data_cobalt_case_study/data_input_cobalt_extended_data_set.xlsx', sh
```

Out[ ]:

	Product categories	distribution	location	scale	shape
0	portable batteries	weibull	0	4.051716	2.09
1	mobility batteries	weibull	0	10.631501	2.20
2	hydroprocessing catalysts coke	weibull	0	2.894742	2.50
3	hydroprocessing catalysts poisoning	weibull	0	1.505266	2.50
4	hydroformylation catalysts	weibull	0	2.315793	2.50
5	pet precursors catalysts	weibull	0	0.578948	2.50
6	dissipative uses	weibull	0	14.435166	3.50
7	hard metals	weibull	0	8.915235	1.16
8	magnets	weibull	0	13.905022	1.93
9	other metallic uses	weibull	0	14.628064	1.47
10	superalloys	weibull	0	17.282543	1.74

In [ ]:
```
pd.read_excel(
    'data_cobalt_case_study/data_uncertainty_rating_cobalt_case_study.xlsx',
    sheet_name='MaTrace_in_use_stock')
```

Out[ ]:

	Product categories	shape	scale
0	portable batteries	0	0
1	mobility batteries	1	4
2	hydroprocessing catalysts coke	2	4
3	hydroprocessing catalysts poisoning	2	4
4	hydroformylation catalysts	2	4
5	pet precursors catalysts	1	4
6	dissipative uses	2	3
7	hard metals	1	2
8	magnets	1	2
9	other metallic uses	1	2
10	superalloys	1	2

As it can be seen, only the uncertainty scores for the columns "shape" and "scale" appear. This is intended since only numerical values can be varied by this implementation and the location of the Weibull distribution is a factor which was not considered.

Once the paths and the settings are defined, the script can be run. The next cell executes the script for 10 runs.

In [ ]:

```
%run monte_carlo_simulations.py
```

```
Creating dictionary for results. Path: monte_carlo_results/proof_of_concept
Importing data
Creating inputs for Monte Carlo simulations based on uncertainty score
Normalize inputs
c:\Users\rapha\Desktop\master_thesis_hand_in\monte_carlo_simulations.py:154: Perfor
manceWarning: indexing past lexsort depth may impact performance.
  for column in input_pd.loc[:, ("MaTrace_initial_inflow", "share")].columns:
Starting runs
Run 1 of 10
Mass balance run 0: True
Run 2 of 10
Mass balance run 1: True
Run 3 of 10
Mass balance run 2: True
Run 4 of 10
Mass balance run 3: True
Run 5 of 10
Mass balance run 4: True
Run 6 of 10
Mass balance run 5: True
Run 7 of 10
Mass balance run 6: True
Run 8 of 10
Mass balance run 7: True
Run 9 of 10
Mass balance run 8: True
Run 10 of 10
Mass balance run 9: True
Total time - seconds: 21,  hours: 0.005833333333333334
```

```
Time per run: 2.1
Inputs and results are stored.
```

The printed output reflects the steps of the code. After the data is imported, random numbers following the defined distributions are created. Since some split vectors and transfer coefficients will not sum up to 1 anymore (see above) they have to be normalized. Afterwards, the experiments are run. The data is collected in a dictionary. If several thousand runs are executed, the dictionary is dumped in splits to decrease the runtime.

The results and a file containing the used model inputs can be found in the folder "monte_carlo_results/proof_of_concept".

The following cell shows part of the saved inputs. The rows represent runs.

In [ ]:

```
import pickle
with open('monte_carlo_results/proof_of_concept/inputs.pkl', 'rb') as f:
    input_pd = pickle.load(f)
input_pd
```

Out[ ]:

sheet column item	portable batteries	mobility batteries	hydroprocessing catalysts coke	hydroprocessing catalysts poisoning	hydroformylation catalysts	pet precursors catalysts	diss
0	0.195626	0.069050	0.049883	0.023999	0.059167	0.004703	0.(
1	0.221689	0.031145	0.057574	0.063652	0.049747	0.142862	0.(
2	0.203971	0.067055	0.028344	0.034823	0.238051	0.132933	0.(
3	0.411710	0.092229	0.039897	0.041033	0.107387	0.019387	0.(
4	0.279781	0.026076	0.036750	0.036071	0.015810	0.016235	0.(
5	0.282791	0.069646	0.045512	0.080305	0.017813	0.049054	0.(
6	0.321172	0.040106	0.077813	0.053932	0.036862	0.058657	0.(
7	0.252250	0.032541	0.046556	0.083294	0.096109	0.016466	0.(
8	0.267555	0.034854	0.015555	0.001666	0.069714	0.074432	0.(
9	0.326831	0.035760	0.133187	0.041984	0.067035	0.004005	0.(

10 rows × 541 columns

The results are saved in the form of nested dictionaries:

In [ ]:

```
with open('monte_carlo_results/proof_of_concept/results.pkl', 'rb') as f:
    results_dic = pickle.load(f)
```

The fist key represents runs:

In [ ]:

```
results_dic.keys()
```

Out[ ]:

```
dict_keys(['0', '1', '2', '3', '4', '5', '6', '7', '8', '9'])
```

The second part specifies from which part of the model the data is coming from:

In [ ]:
```
results_dic['0'].keys()
```

Out[ ]:
```
dict_keys(['matrace_data_dic', 'reuse_data_dic'])
```

Since this data structure is hard to handle, the script "monte_carlo_evaluation.py" serves the purpose to transfer the data into multidimensional pandas data frames.

Executing "monte_carlo_evaluation.py"

In order to execute this script, one has to adjust the settings in the beginning of the file so they are the same as the used ones in "mone_carlo_simulations.py". The path to the results has to be defined. Then the file is ready to be executed.

In [ ]:
```
%run monte_carlo_evaluation.py
```

```
Loading file:
Create dictionary:
Start treating data
run 1 of 10
run 2 of 10
run 3 of 10
run 4 of 10
run 5 of 10
run 6 of 10
run 7 of 10
run 8 of 10
run 9 of 10
run 10 of 10
Compact results are stored.
```

This script creates the multidimensional pandas data frame 'compact_results'. The first key entails the runs, the second the stock or flow, and the third one the product or the product category.

In [ ]:
```
with open('monte_carlo_results/proof_of_concept/compact_results.pkl',
    'rb') as f:
    compact_results = pickle.load(f)
compact_results
```

Out[ ]:

run									
stock_flow								**total_use_stock**	**t**
item	**sum**	**smartphones**	**mobile phones**	**tablets**	**laptops**	**e-bikes**	**power tools**	**others**	
2015	0.195626	0.057242	0.047268	0.02614	0.048304	0.001794	0.006937	0.007942	
2016	0.177952	0.053884	0.036155	0.02468	0.047307	0.001774	0.006729	0.007423	0.01
2017	0.1475	0.046705	0.021888	0.020836	0.044188	0.001634	0.006348	0.005901	0.02
2018	0.116835	0.037369	0.012804	0.015898	0.039273	0.001304	0.005903	0.004284	0.04
2019	0.090162	0.027998	0.008145	0.011246	0.033273	0.000864	0.005448	0.003187	0.04

run									
stock_flow								total_use_stock	t
item	sum	smartphones	mobile phones	tablets	laptops	e-bikes	power tools	others	
2020	0.069089	0.020143	0.006213	0.007728	0.027022	0.000502	0.005007	0.002473	0.04
2021	0.053197	0.01421	0.00547	0.005481	0.021222	0.000322	0.00459	0.001902	0.04
2022	0.041158	0.009933	0.004847	0.004179	0.016291	0.000263	0.004195	0.00145	0.03
2023	0.031819	0.006883	0.003998	0.003389	0.012354	0.000232	0.003823	0.001141	0.03
2024	0.024471	0.004703	0.003038	0.002799	0.009323	0.000194	0.003472	0.000942	0.02
2025	0.01869	0.003151	0.002168	0.002264	0.007016	0.00015	0.003139	0.000802	0.02
2026	0.014169	0.002059	0.001487	0.001757	0.005248	0.000108	0.002824	0.000686	0.01
2027	0.010659	0.00131	0.000997	0.001299	0.003875	0.000073	0.002528	0.000577	0.01
2028	0.007954	0.000811	0.000655	0.000915	0.002804	0.000046	0.00225	0.000472	0.00
2029	0.005892	0.000489	0.00042	0.000614	0.001976	0.000027	0.001991	0.000375	0.00
2030	0.004344	0.000287	0.00026	0.000393	0.001349	0.000015	0.001752	0.000288	0.00
2031	0.003204	0.000165	0.000153	0.00024	0.000891	0.000008	0.001532	0.000213	0.00
2032	0.002377	0.000092	0.000086	0.00014	0.000569	0.000004	0.001332	0.000153	0.00
2033	0.001785	0.00005	0.000046	0.000078	0.000351	0.000002	0.001152	0.000106	0.00
2034	0.001363	0.000027	0.000023	0.000042	0.00021	0.000001	0.00099	0.000071	0.00
2035	0.001061	0.000014	0.000011	0.000021	0.000121	0.0	0.000847	0.000046	0.00
2036	0.00084	0.000007	0.000005	0.00001	0.000068	0.0	0.000721	0.000029	0.00
2037	0.000675	0.000004	0.000002	0.000005	0.000037	0.0	0.00061	0.000018	0.00
2038	0.000549	0.000002	0.000001	0.000002	0.000019	0.0	0.000515	0.00001	0.00
2039	0.00045	0.000001	0.0	0.000001	0.00001	0.0	0.000432	0.000006	0.00
2040	0.000371	0.0	0.0	0.0	0.000005	0.0	0.000361	0.000003	0.00
2041	0.000306	0.0	0.0	0.0	0.000002	0.0	0.000301	0.000002	0.00
2042	0.000252	0.0	0.0	0.0	0.000001	0.0	0.00025	0.000001	0.00
2043	0.000208	0.0	0.0	0.0	0.000001	0.0	0.000207	0.000001	0.00
2044	0.000171	0.0	0.0	0.0	0.0	0.0	0.000171	0.0	0.00
2045	0.000141	0.0	0.0	0.0	0.0	0.0	0.00014	0.0	0.00
2046	0.000115	0.0	0.0	0.0	0.0	0.0	0.000115	0.0	0.00
2047	0.000094	0.0	0.0	0.0	0.0	0.0	0.000094	0.0	0.00
2048	0.000077	0.0	0.0	0.0	0.0	0.0	0.000077	0.0	0.00
2049	0.000063	0.0	0.0	0.0	0.0	0.0	0.000063	0.0	0.00
2050	0.000051	0.0	0.0	0.0	0.0	0.0	0.000051	0.0	0.00

36 rows × 5240 columns

Executing "monte_carlo_uncertainty.py"

In order to execute this script, one has to adjust the settings in the beginning of the file so they are the same as the used ones in "mone_carlo_simulations.py" and "monte_carlo_evaluation.py". The path to the results has to be defined. Then the file is ready to be executed.

The file calculates for all considered years the spearman correlation and the normalized spearman square correlation between all inputs and the total in-use stock, the total hibernating stock, the total disposal flow, and the total export flow.

The results are written into the files "monte_carlo_results" (results of mentioned stocks and flows over years and runs), "speaman_results_abs" (spearman correlation between inputs and outputs over years) and "spearman_results_normalized" (normalized spareman square correlation between inputs and outputs over years).

In [ ]:

```
%run monte_carlo_uncertainty.py
```

```
Calculate spearman correlation between inputs and:
['total_use_stock', 'total_hoarding_stock', 'to_disposal_flow', 'U.B hoarding stoc
k', 'U.A use stock', 'total_export', 'total_disposal']
Year 1 of 36
c:\Users\rapha\.conda\envs\master_thesis\lib\site-packages\scipy\stats\stats.py:448
4: SpearmanRConstantInputWarning: An input array is constant; the correlation coeff
icient is not defined.
  warnings.warn(SpearmanRConstantInputWarning())
Year 2 of 36
Year 3 of 36
Year 4 of 36
Year 5 of 36
Year 6 of 36
Year 7 of 36
Year 8 of 36
Year 9 of 36
Year 10 of 36
Year 11 of 36
Year 12 of 36
Year 13 of 36
Year 14 of 36
Year 15 of 36
Year 16 of 36
Year 17 of 36
Year 18 of 36
Year 19 of 36
Year 20 of 36
Year 21 of 36
Year 22 of 36
Year 23 of 36
Year 24 of 36
Year 25 of 36
Year 26 of 36
Year 27 of 36
Year 28 of 36
Year 29 of 36
Year 30 of 36
Year 31 of 36
Year 32 of 36
```

```
Year 33 of 36
Year 34 of 36
Year 35 of 36
Year 36 of 36
Export Monte Carlo results
Export spearman absolute results
Export spearman normalized results
```

The following cell shows a part of the table displaying the normalized square spearmen correlation.

In [ ]:

```python
with open(
    'monte_carlo_results/proof_of_concept/spearman_results_normalized.pkl',
     'rb') as f:
    spearman_results_normalized_pd= pickle.load(f)
spearman_results_normalized_pd
```

Out[ ]:

result_item sheet column item	portable batteries	mobility batteries	hydroprocessing catalysts coke	hydroprocessing catalysts poisoning	hydroformylation catalysts	pet precursors catalysts
0	2.045029	0.114251	0.081801	0.138889	0.033126	0.138889
1	1.986973	0.039561	0.062895	0.081441	0.039561	0.179560
2	1.887136	0.012615	0.032919	0.021573	0.012615	0.151159
3	1.887136	0.012615	0.032919	0.021573	0.012615	0.151159
4	1.887136	0.012615	0.032919	0.021573	0.012615	0.151159
5	1.949861	0.081918	0.021740	0.039793	0.009102	0.195656
6	1.949861	0.081918	0.021740	0.039793	0.009102	0.195656
7	1.956062	0.228274	0.021809	0.055012	0.000679	0.092442
8	1.812508	0.063447	0.001886	0.000075	0.009129	0.103281
9	1.887136	0.012615	0.032919	0.021573	0.012615	0.151159
10	1.769097	0.000663	0.005964	0.008910	0.021281	0.206843
11	1.643312	0.001850	0.001850	0.003627	0.053960	0.177721
12	1.331594	0.053264	0.038651	0.003580	0.089504	0.190040
13	1.331594	0.053264	0.038651	0.003580	0.089504	0.190040
14	1.305751	0.021333	0.090426	0.021333	0.039049	0.207352
15	1.049711	0.001853	0.352918	0.101480	0.026760	0.071236
16	1.049711	0.001853	0.352918	0.101480	0.026760	0.071236
17	1.049711	0.001853	0.352918	0.101480	0.026760	0.071236
18	1.200942	0.012583	0.334245	0.091212	0.000670	0.054280
19	0.971130	0.033540	0.549488	0.182605	0.040232	0.012853
20	1.022361	0.209790	0.442806	0.062810	0.054445	0.000075

result_item						
sheet						
column						
item	**portable batteries**	**mobility batteries**	**hydroprocessing catalysts coke**	**hydroprocessing catalysts poisoning**	**hydroformylation catalysts**	**pet precursors catalysts**
21	1.079578	0.292661	0.351060	0.012461	0.021310	0.001843
22	1.079578	0.292661	0.351060	0.012461	0.021310	0.001843
23	0.962534	0.424015	0.379993	0.016961	0.092341	0.003694
24	0.893307	0.569097	0.400676	0.054812	0.102932	0.006090
25	0.893307	0.569097	0.400676	0.054812	0.102932	0.006090
26	0.752894	0.666098	0.274632	0.000664	0.311830	0.001845
27	0.752894	0.666098	0.274632	0.000664	0.311830	0.001845
28	0.880273	0.697121	0.136994	0.003630	0.294067	0.026747
29	0.880273	0.697121	0.136994	0.003630	0.294067	0.026747
30	0.880273	0.697121	0.136994	0.003630	0.294067	0.026747
31	0.880273	0.697121	0.136994	0.003630	0.294067	0.026747
32	0.779623	0.663220	0.123532	0.016535	0.176442	0.021238
33	0.779623	0.663220	0.123532	0.016535	0.176442	0.021238
34	0.779623	0.663220	0.123532	0.016535	0.176442	0.021238
35	0.779623	0.663220	0.123532	0.016535	0.176442	0.021238

36 rows × 3787 columns

Using this data, one can create plots displaying the contribution of an input to the uncertainty of an output. The following graph is not representative since only 10 runs were conducted.

In [ ]:

```
graph_pd = spearman_results_normalized_pd.groupby(level=[0,1,2], axis = 1).sum()

graph_pd = graph_pd['U.A use stock'].copy()
graph_pd.columns = ['_'.join(col) for col in graph_pd.columns]
graph_pd


dic_legend = {'n_initial_products_Share': r'$\eta$: Initial inflow distribution',
'n_use_1_in_use_Weibull scale': r'$S_{Uk}$: Weibull scale',
'n_use_1_in_use_Weibull shape': r'$S_{Uk}$: Weibull shape',
'reuse_split_split': r'$\delta$: Split portable batteries to products'
}
handles_names_list = []

fig, ax = plt.subplots()
stacks = ax.stackplot(graph_pd.index, graph_pd.transpose().to_numpy())

plt.ylabel('Normalized square of Spearman\'s rank correlation in %')
plt.xlabel('Year')
```

Out[ ]: Text(0.5, 0, 'Year')