Habilitationsschrift

Analyse, Bewertung und Gestaltung von Materialkreisläufen

Habilitation thesis

Analysis, Evaluation and Design of Material Cycles

vorgelegt zum Zwecke der Erlangung der Lehrbefugnis
für das Fach
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Kurzfassung

Der Übergang von linearen Modellen der Ressourcennutzung zu vermehrter Kreislaufwirtschaft beinhaltet Maßnahmen zur Reduktion, Wiederverwendung, materiellen Verwertung, thermischen Verwertung und sicheren Ablagerung von Abfällen. Da Abfälle als Rohstoffe genutzt werden können, aber auch gefährliche Stoffe enthalten können, stellt die Identifikationen optimaler abfallwirtschaftlicher Lösungen ein komplexes Unterfangen dar, das eine systemische Sichtweise bedingt. In diesem Zusammenhang bildet das Verständnis der Materialflüsse und Materiallager in der Gesellschaft eine wesentliche Grundlage für die Bewertung von Abfall- und Ressourcensystemen, welche durch eine Materialflussanalyse (MFA) geschaffen wird. Die Umweltrelevanz der Abfall- und Ressourcenflüsse über den gesamten Lebenszyklus (von der Rohstoffgewinnung bis zur endgültigen Ablagerung) kann anhand einer Ökobilanz (engl.: Life Cycle Assessment, LCA) ermittelt werden. Daher stellt die Kombination von MFA und LCA eine ideale Entscheidungsgrundlage für die Gestaltung ökologisch optimaler Abfall- und Ressourcensysteme dar. Die gegenständliche Arbeit besteht aus einer Reihe von Publikationen, die drei zentrale Bereiche der Analyse, Bewertung und Gestaltung von Materialkreisläufen behandeln. Erstens, den Umgang mit Unsicherheiten in MFA, der wesentlich für die Schaffung einer robusten Entscheidungsbasis ist. Zweitens, die Modellierung dynamischer Ressourcensysteme, um den Effekt bestimmter Maßnahmen und Szenarien auf Flüsse und Lager von Materialien zu bestimmen. Drittens, die Bewertung von Ressourcennutzungsstrategien auf unterschiedlichen Ebenen, da diese grundlegend für die Gestaltung von Abfall- und Ressourcensystemen aus ökologischer Sicht ist. Der Großteil der wissenschaftlichen Publikationen dieser Arbeit liegt im Bereich der Materialflussanalyse, wo methodische Beiträge entwickelt (Unsicherheits- und Sensitivitätsanalyse, dynamische Modellierung) und in Fallstudien angewendet wurden. Außerdem gelangen bei der Kombination von MFA und Wirkungsabschätzungsmethoden bedeutende Fortschritte. In erster Linie konnten durch die Kombination von MFA und LCA die Umweltauswirkungen von Material- und Energieflüssen des untersuchten Ressourcensystems ermittelt werden. Zudem wurden Exergie und statistische Entropie als Effizienzmaße für Ressourcensysteme evaluiert. Dementsprechend stellt diese Arbeit, neben den Errungenschaften im MFA-Bereich, einen Schritt zur Integration von MFA und LCA als Basis für nachhaltiges Abfall- und Ressourcenmanagement dar. Der Übergang zu stärkerer Kreislaufwirtschaft wird die Abhängigkeit zwischen Altmaterialien und Produktionsrohstoffen in Zukunft verstärken, wodurch sich weiterer Forschungsbedarf ergibt. In Bezug auf den Umgang mit Unsicherheiten in MFA sollte der Fokus auf der Implementierung der entwickelten Methoden in benutzerfreundlichen Lösungen für MFA-Anwender liegen. Im Rahmen der Modellierung von Materialkreisläufen wird die gleichzeitige Betrachtung von Stoff-, Güter- und Produktebenen an Bedeutung gewinnen, um Qualitätsaspekte besser abbilden zu können. Schließlich ist auch eine weitere Integration von MFA und LCA anzustreben, die ein systemisches Verständnis kritischer Faktoren für die Umweltrelevanz von Abfall- und Ressourcensystemen begründen können.

Abstract

The transition from linear-type use and dispose economies to more circular models of resource use entails measures to reduce, reuse, recycle, energetically valorize, and safely dispose of wastes. Because wastes can serve as resources in different production systems and may contain hazardous materials, identifying optimal waste solutions is a complex task, which requires a systems perspective. Material flow analysis (MFA) is typically applied to analyze the flows and stocks of materials in society. It provides the basis for assessing different waste and resource management solutions by mapping the respective flows of materials and energy. The environmental performance of a waste system can be evaluated using life cycle assessment (LCA), which assesses impacts on the environment resulting from the provision of products and services, taking into account the whole life cycle of the product. Thus, in combination, MFA and LCA represent the framework for sound and comprehensive decision support on designing environmentally optimal waste and resource systems. The present thesis consists of a series of scientific articles, which contribute to three key domains of the analysis, evaluation and design of material cycles. First, the handling of uncertainty in MFA, which is crucial for robust decision support on waste and resource systems. Second, the modeling of resource system dynamics, which is required to evaluate the effect of specific measures or scenario settings on material stocks and flows. Third, the evaluation of resource recovery strategies on different levels as a basis for environmentally optimal design of waste and resource systems. The majority of the scientific articles in this thesis focused on the MFA domain, where significant methodological developments could be achieved (e.g. uncertainty and sensitivity analysis, dynamic modeling) and illustrated via case studies. However, research was also progressed regarding the combination of MFA with impact assessment methods. In particular, with LCA to determine environmental impacts associated with the material and energy flows of the resource system under investigation. In addition, exergy and statistical entropy methods were applied on top of MFA to test them as resource efficiency indicators for macro-scale material flow systems. Hence, in addition to the achievements in the MFA domain, the thesis represents a major step towards the integration of MFA and LCA in a holistic framework for environmental decision support on waste and resource management. In the future, the transition towards more circular material flow systems will further increase the interdependency between end-of-life (EOL) flows and inputs to the production systems, requiring research efforts in each of the topical areas addressed in this thesis. Concerning the handling of uncertainty in MFA, the focus should shift from method development to the implementation of state-of-the-art methods via easy-to-use tools for MFA practitioners. Given increasing shares of secondary production, the simultaneous modeling of substance, goods, and product cycles in dynamic MFA will evolve as a major field of future research to reflect the quantity and quality dimension of material cycles. Finally, further efforts are also required to integrate MFA and LCA models in consistent modeling frameworks to create a systemic understanding of the role of specific factors and conditions for the environmental performance of waste and resource systems.

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1 Introduction

1.1 Motivation and background

In Europe as well as around the globe increasing resource efficiency to enable sustainable economies is a pressing issue (cf. EC 2011). The transition towards a more circular economy is seen as a key element to achieve a high degree of resource efficiency (cf. EC 2014, 2015). It aims at material cycles, where waste is minimized and turned into resources, which can be used in production processes and thereby increase overall resource productivity. Environmental impacts often decrease with increasing circularity, but there are also tipping points at which, for example, the additional impact of an increasing energy demand per unit of recovered material is higher than the gains. Such trade-offs need to be considered when designing circular material flow systems. Moreover, to achieve circular material flow systems, systemic changes are required in different areas ranging from specific technology developments to large-scale societal changes (Bocken et al. 2017). Therefore, the definition of suitable strategies for increasing the resource efficiency of material flow systems requires a holistic perspective, taking into account direct impacts of material use but also indirect consequences, such as effects on other resource systems, for example, due to product substitution (cf. Laurent et al. 2014a.). Thus, decision support tools need to be based on consistent and comprehensive modeling approaches, reflecting the complex relationships and constraints of a specific resource system as well as its interaction with other resource systems.

Material flow analysis (MFA) quantifies the flows and stocks of materials in arbitrarily complex systems (Brunner and Rechberger 2004) and has been widely applied to resource systems providing useful information regarding the patterns of resource use and the losses of materials entering the environment (Chen and Graedel 2012a). However, MFA does not directly inform about the environmental relevance of the different material flows. LCA is therefore often used to evaluate impacts on the environment resulting from the provision of products and services, taking into account the whole life cycle of the product from raw material acquisition to final disposal or secondary production (ISO 2006). In the field of waste and resource management, state-of-the-art environmental assessments often apply MFA and LCA in combination, to guarantee for consistent inventory data, on the one hand, and to capture environmental impacts of waste management outside the main system, on the other hand (e.g. Tonini et al. 2013, Vadenbo et al. 2014). Thus, the combination of MFA and LCA offers the potential for more consistent and reliable decision support in environmental and resource management by simultaneously taking into account material efficiencies and environmental impacts. Constraints that are normally not accounted for in LCA, such as limited production capacity or dynamics in (secondary) raw material supply (quantitative and qualitative), can be considered using material flow models (Laner and Rechberger 2016). LCA, on the other hand, can be used to identify preferable alternatives

for resource use from an environmental perspective offering a wide range of impact categories (e.g. Laurent et al. 2014b).

Circular material flow systems avoid wastes and use end-of-life material flows as resources for secondary production. To increase the extent of material cycling by enhanced use of obsolete material stocks and flows as resources, an understanding of the whole resource system with respect to the quantity and quality of secondary raw materials is essential (cf. Lederer et al. 2014). In order to designate obsolete materials as resources and re-introduce them into the product cycle, various challenges need to be addressed:

i) A crucial part of the knowledge base for resource recovery is reliable information on waste composition and treatment as well as recovery processes. Such information can be generated by direct waste sampling and analysis (e.g. Skutan and Brunner 2012), monitoring of waste management processes (e.g. Morf and Brunner 1998), plant-level MFA (e.g. Velis et al. 2013), and macro-scale MFA (e.g. Moriguchi and Hashimoto 2016). Because each approach has specific limitations, a combination of methods (e.g. determining waste composition based on representative sampling and MFA-based predictions of obsolete material flows) is most suitable to determine the resource potential of a specific material flow. In any case, the complexity of products and the heterogeneity of waste streams only allow for estimates about the quantity of anthropogenic resources available, which makes the amounts of potentially recoverable materials inherently uncertain.

ii) Another critical aspect of resource recovery is the functionality of end-of-life (EOL) materials with respect to their use as secondary raw materials and the interaction between secondary production and primary (or traditional) production routes. Therefore, an understanding of the whole resource system needs to be generated and system dynamics have to be considered (e.g. changes in regulations concerning substance use in products, changes in product use patterns, etc.). This can be achieved by comprehensive dynamic material flow analyses, which allow for analyzing the quantitative (i.e. related to mass) and qualitative (i.e. contaminants and technical material qualities such as metal alloy mixtures) aspects of material recycling (e.g. for the global steel cycle: Nakamura et al. 2014, Nakamura et al. 2017, Pauliuk et al. (2017)). In view of increasingly circular material flow systems, considering substance concentrations and technical properties in dynamic material flow models has become increasingly important to understand the role of anthropogenic material stocks and EOL flows as part of the resource base of modern society.

iii) Finally, recovery strategies and recycling schemes need to be evaluated with respect to central dimensions of resource use (costs, environmental impacts, supply security, etc.) to identify optimal system designs and solutions. Therefore, comprehensive material resource efficiency indicators are needed (e.g. recycling rates, open- vs. closed-loop recycling, share of secondary production, etc.), which allow for meaningful comparisons concerning the circularity of resource systems (cf. Chen 2013, Haupt et al. 2017). Although policies are often based on material-

efficiency targets such as recycling rates (e.g. circular economy package of the Europen Union), decision support on optimal resource system design needs to be based on environmental impacts rather than on material circularity. Hence, determining the environmental impacts of resource recovery and recycling schemes is essential to identify environmentally optimal recycling strategies and system configurations. Consequently, the material and the environmental dimensions of resource systems need to be integrated in order to provide sound decision support for resource systems design.

The above challenges (i – iii) related to resource recovery strategies and the stimulation of material cycles are central aspects of the analysis, evaluation and design of material cycles. Therefore, they motivated this thesis and many of these aspects are addressed by the research constituting this work.

1.2 Scope and structure of the thesis

The present thesis is based on 17 scientific publications (see appendix), which contribute to three key domains of the analysis, evaluation and design of material cycles: First, the handling of uncertainty in MFA, which is crucial for the analysis of waste and resource systems; second, the modeling of resource system dynamics, which is required to evaluate the effect of specific measures or scenario settings on material stocks and flows; and third, the evaluation of resource recovery strategies on different levels from waste- or technology-specific assessments to national or regional assessments of a specific resource or a specific sector, which is the basis for environmentally optimal systems design. The three domains and the individual publications within each domain are listed below. In Chapter 2, the main contributions of each publication are described and major innovations are highlighted. In Chapter 3, the findings of this thesis are summarized and an outlook on future research is provided.

Handling uncertainty in Material Flow Analysis (cf. chapter 2.1)

[1] **Laner, D.**, Rechberger, H. and Astrup, T. (2014) Systematic Evaluation of Uncertainty in Material Flow Analysis. Journal of Industrial Ecology 18(6), 859-870.

[2] Schwab, O., **Laner, D.** and Rechberger, H. (2017) Quantitative Evaluation of Data Quality in Regional Material Flow Analysis. Journal of Industrial Ecology 21(5), 1068-1077.

[3] **Laner, D.**, Feketitsch, J., Rechberger, H. and Fellner, J. (2016) A Novel Approach to Characterize Data Uncertainty in Material Flow Analysis and its Application to Plastics Flows in Austria. Journal of Industrial Ecology 20(5), 1050-1063.

[4] **Laner, D.**, Rechberger, H. and Astrup, T. (2015) Applying Fuzzy and Probabilistic Uncertainty Concepts to the Material Flow Analysis of Palladium in Austria. Journal of Industrial Ecology 19(6), 1055-1069.

[5] Džubur, N., Sunanta, O. and **Laner, D.** (2017) A fuzzy set-based approach to data reconciliation in material flow modeling. Applied Mathematical Modelling 43, 464-480.

[6] Džubur, N., Buchner, H. and **Laner, D.** (2017) Evaluating the Use of Global Sensitivity Analysis in Dynamic MFA. Journal of Industrial Ecology 21(5), 1212-1225.

[7] Klinglmair, M., Zoboli, O., **Laner, D.**, Rechberger, H., Astrup, T.F. and Scheutz, C. (2016) The effect of data structure and model choices on MFA results: A comparison of phosphorus balances for Denmark and Austria. Resources, Conservation and Recycling 109, 166-175.

Analysis of resource system dynamics (cf. chapter 2.2)

[8] Buchner, H., **Laner, D.**, Rechberger, H. and Fellner, J. (2015) Dynamic Material Flow Modeling: An Effort to Calibrate and Validate Aluminum Stocks and Flows in Austria. Environmental Science & Technology 49(9), 5546-5554.

[9] Buchner, H., **Laner, D.**, Rechberger, H. and Fellner, J. (2015) Future Raw Material Supply: Opportunities and Limits of Aluminium Recycling in Austria. Journal of Sustainable Metallurgy 1(4), 253-262.

[10] Džubur, N. and **Laner, D.** (2017) Evaluation of Modeling Approaches to Determine End-of-Life Flows Associated with Buildings: A Viennese Case Study on Wood and Contaminants. Journal of Industrial Ecology.

[11] Buchner, H., **Laner, D.**, Rechberger, H. and Fellner, J. (2017) Potential recycling constraints due to future supply and demand of wrought and cast Al scrap—A closed system perspective on Austria. Resources, Conservation and Recycling 122, 135-142.

[12] Pivnenko, K., **Laner, D.** and Astrup, T.F. (2016) Material Cycles and Chemicals: Dynamic Material Flow Analysis of Contaminants in Paper Recycling. Environmental Science & Technology 50(22), 12302-12311.

Evaluation of resource recovery strategies (cf. chapter 2.3)

[13] **Laner, D.** and Rechberger, H. (2007) Treatment of cooling appliances: Interrelations between environmental protection, resource conservation, and recovery rates. Resources, Conservation and Recycling 52(1), 136-155.

[14] Huber, F., **Laner, D.** and Fellner, J. (2017) Comparative life cycle assessment of MSWI fly ash treatment and disposal. Waste Management.

[15] **Laner, D.**, Cencic, O., Svensson, N. and Krook, J. (2016) Quantitative Analysis of Critical Factors for the Climate Impact of Landfill Mining. Environmental Science & Technology 50(13), 6882-6891.

[16] **Laner, D.**, Rechberger, H., De Soete, W., De Meester, S. and Astrup, T.F. (2015) Resource recovery from residual household waste: An application of exergy flow analysis and exergetic life cycle assessment. Waste Management 46, 653-667.

[17] **Laner, D.**, Zoboli, O. and Rechberger, H. (2017) Statistical entropy analysis to evaluate resource efficiency: Phosphorus use in Austria. Ecological Indicators 83(Supplement C), 232-242.

2 Scientific achievements

The significance of the three domains for the analysis, evaluation and design of material cycles as well as the individual contributions made by this thesis to each domain are described in this chapter.

2.1 Handling uncertainty in Material Flow Analysis

Material flow analysis (MFA) is a tool to evaluate material use patterns by quantifying stocks and flows in a temporally and geographically defined system (Baccini and Brunner 1991, Brunner and Rechberger 2016). Like any other model-based decision support tool, MFA results are inherently uncertain. Due to varying data quality, limited data availability, and lack of system understanding, the true quantities of material stocks and flows are unknown and need to be estimated. In the past, these estimates were often presented as nominal values, which raised doubts about the credibility of MFA results (cf. Danius and Burström 2001, Montangero and Belevi 2007, Rechberger et al. 2014). Therefore, recently efforts have been made to systematically address vagueness and uncertainty in MFA and quantify its effect on MFA-based decision support for environmentally sound resource use. In essence, three subsequent steps of uncertainty analysis can be distinguished in MFA (see Figure 1):

- **In the first step**, the quality of MFA input data is assessed and input uncertainties are characterized. The major idea of this step is to translate data deficiencies into specific mathematical functions, which express the degree of belief that the input value captures the true value of the quantity of interest. In the past, little research was done with a focus on the systematic evaluation of MFA input data uncertainty, although many studies highlighted the crucial importance of data quality for the reliability of MFA results (cf. Graedel et al. 2004, Rechberger et al. 2014). Therefore, several of the studies constituting this thesis put a focus on this issue by discussing or applying existing methods ([*1], [4], [5]*) or even developing novel frameworks for data quality assessment and uncertainty characterization (*[2], [3]*). Because this step is and will remain the most subjective element of uncertainty analysis in MFA, establishing transparent and consistent procedures for documentation and evaluation of MFA data quality as well as for characterization of MFA input uncertainty is crucial for reliable MFA-based decision support.
- **In the second step**, the input data are fed into the material flow model. If the number of unknown variables (= no input data available) is smaller than the number of balance equations (i.e. each process of the material flow model represents a balance volume), inconsistencies between input data may arise given the mass balance constraints of the model. Provided that flows are defined as uncertain variables, procedures for reconciling conflicting input data can be applied and the resulting flow uncertainties are propagated in the model. Traditionally, data

reconciliation and error propagation procedures were based on the assumption of independently determined flow variables with random, i.e. normally distributed, estimation errors (cf. Baccini and Bader 1996). This is the case in the most widely used MFA software, STAN (Cencic and Rechberger 2008), where data reconciliation is based on a least-squares approach using a Gauss-Jordan elimination process (Cencic 2016) and the uncertainty of the results is derived via Gaussian error propagation. However, due to limitations inherent in the assumption of normally distributed variables (e.g. lack of empirical data to derive density functions, density function is symmetric around the mean, negative values cannot be excluded), recent efforts have been made to develop methods, which allow for more flexibility in the definition of input uncertainty (e.g. Bornhöft et al. 2016, Cencic and Frühwirth 2015, Dubois et al. 2014, Gottschalk et al. 2010, Kopec et al. 2015, Lupton and Allwood 2017). Major contributions have also been made in this thesis, by systemizing existing procedures and their fields of application (cf. *[1]*) and, in particular, by developing methods based on possibility theory to express and handle uncertainty in MFA (*[4]*, *[5]*).

- **In the third step,** MFA results are interpreted and the uncertainty is communicated. In most cases, uncertainty ranges are used to express the range of values including the true value with a certain (pre-defined) probability (e.g. 95%) and flow values are rounded to significant digits (cf. Rechberger et al. 2014). Many studies refrain from more detailed analysis and interpretation of the results' uncertainty. However, in view of the diverse sources of uncertainty more critical analysis and discussion seems appropriate. First, one should be aware of the ignorance in uncertainty analysis concerning model and scenario uncertainty, which is related to modeler's choices on model structure, data types and sources, and mathematical procedures in the model. This was addressed in *[7]*, and is, apart from this study, generally ignored in the MFA literature. Second, the analysis of the data reconciliation procedure offers a means to evaluate the plausibility of MFA results (consistency between independent input data in view of mass balance constraints of the model) and thereby indicate the quality of the material flow balance. This kind of analysis is illustrated in *[5]* by exploring trade offs between confidence in input data and consistency within the material flow model and by visualizing the resulting consistency levels for each flow in the material flow diagram. Finally, efforts should also be made to understand the effect of assumptions and input uncertainties on the model outcomes. This is of particular relevance in case of MFA studies, which aim to investigate the effect of changes in different input variables on specific output variables (i.e. typical in dynamic MFA). Although scenario analysis and sensitivity analysis have been applied to investigate these effects (e.g. Glöser et al. 2013, Müller et al. 2014, Pauliuk et al. 2013, Schaffner et al. 2009), this has mostly been done using mathematically simple methods only for selected parameters or settings. Therefore, an approach for decomposing the uncertainty of dynamic MFA results into fractions related to the uncertainty of specific parameters (=input variables) is

presented in *[6]* and used to develop a decision scheme for choosing appropriate sensitivity analysis methods in dynamic MFA studies.

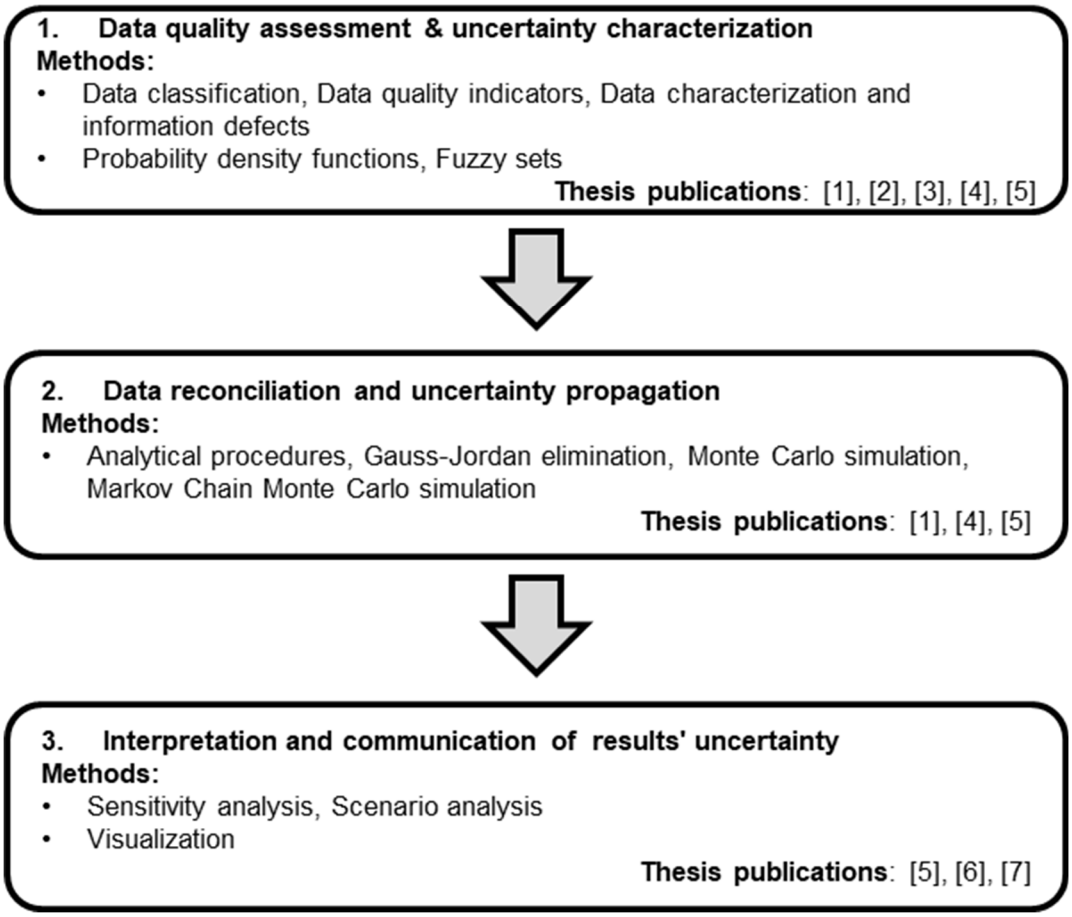

Figure 1: Major steps of handling uncertainty in Material Flow Analysis and related publications of this thesis

2.1.1 Systematic evaluation of uncertainty in MFA (*Publication [1]*)

The aim of the study was to review and assess uncertainty analysis practices in MFA and to develop a protocol for consistent uncertainty treatment in MFA studies. Therefore, various approaches of handling uncertainty in MFA and related fields (i.e. life cycle inventory modeling) were investigated and classified into three groups: (i) qualitative and semi-quantitative approaches; (ii) approaches based on data classification; and (iii) statistical approaches. (i) Qualitative and semi-quantitative approaches are relatively simple and use categories to express the uncertainty of MFA results, e.g. confidence ratings (cf. Graedel et al. 2004) or uncertainty scales (cf. Andersson et al. 2012). (ii) Data classification approaches focus on the characterization of input data and can be based on few criteria (e.g. data source-oriented concept by Hedbrant and Sörme (2001)) or several indicators (e.g. data quality indicators of the Pedigree matrix by Weidema and Wesnæs (1996)). Appropriate procedures for reconciling and propagating data uncertainty in the material flow model are not specified or based on simplifying assumptions. (iii) In statistical approaches,

uncertain variables are defined as probability density functions (e.g. Cencic and Frühwirth 2015, Gottschalk et al. 2010, Montangero and Belevi 2007) or membership functions (e.g. Clavreul et al. 2013, Dubois et al. 2014) and mathematical methods are used to determine the uncertainty of model results.

The critical review of the established practice of uncertainty analysis in MFA highlighted that many MFA studies treated uncertainty, if at all, in a cursory fashion. This resulted in inconsistencies concerning assumptions underlying uncertainty analysis methods and lacking transparency, which undermined the credibility of MFA results. Hence, a step-wise procedure was developed based on the reviewed studies to facilitate consistent and transparent uncertainty handling in MFA (see Figure 2). The first step is part of the system definition step in the overall MFA method (cf. Brunner and Rechberger 2004) and depends on the goal and scope of the MFA. In the second step, the quality of input data is assessed and translated into characterizing functions for mathematical treatment in the material flow model. In the third step, the input data is combined with the model (i.e. balance constraints of the various processes considered in the model) and model results are calculated. In case of over-determined equation systems (i.e. less unknown variables than balance equations) or if independent estimates for specific flows are available, several loops of improving the database and adjusting assumptions are typically required to achieve plausible model results. Subsequently (fourth step in Figure 2), the, so-called, calibrated model is used to derive and visualize the final MFA results. This is typically the last step for descriptive MFA, where the main aim is to quantify the material turnover in a region (i.e. establishing a resource budget). For exploratory MFA studies, which mainly aim at modeling system behavior, sensitivity and/or scenario analysis are performed in the fifth step to identify critical model parameters and to evaluate the effect of specific measures on material flows and stocks.

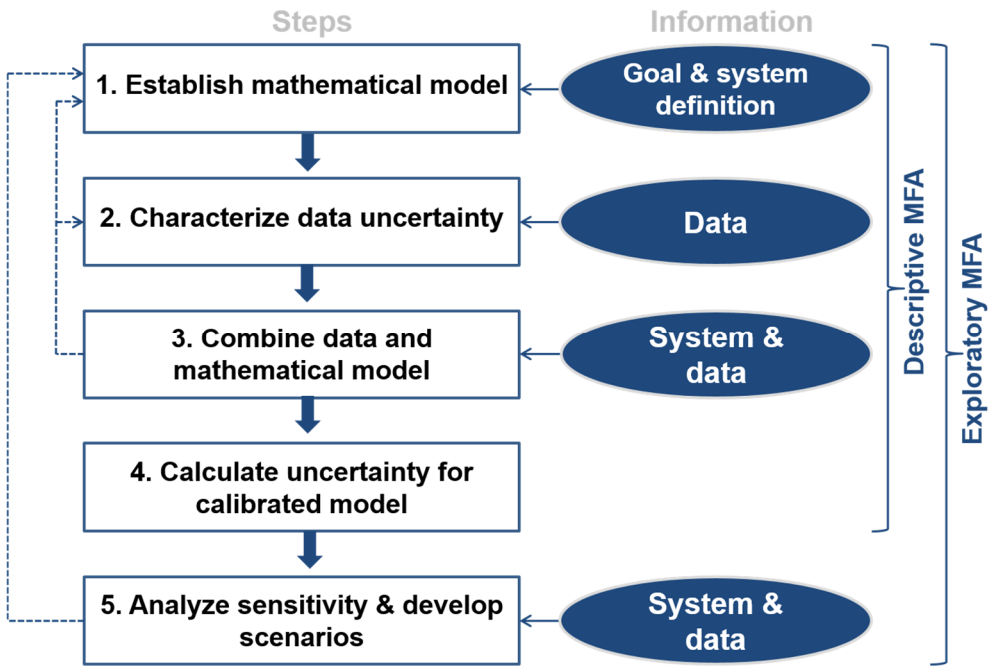

Figure 2: Procedure to treat uncertainty in MFA (adapted from [1])

The major achievements of this study were the systematic analysis of the existing practice of uncertainty consideration in MFA and the definition of a framework, which created a basis for distinguishing individual steps of uncertainty analysis and evaluating available methods for data quality assessment, uncertainty characterization, data reconciliation as well as uncertainty propagation. Therefore, this study prepared the ground for using all the available information on a material flow system in MFA in a consistent and transparent manner and, thereby, produce MFA results as precise as the available data warrant. Major research needs were identified concerning the translation of data quality into uncertainty estimates and the use of different concepts (probabilistic vs. possibilistic) for uncertainty representation and propagation according to the nature (aleatory vs. epistemic) of uncertainty.

2.1.2 Quantitative evaluation of data quality in MFA (*Publication [2]*)

The study presented in *[2]* reflected the finding of *[1]* that the lack of information about input data poses a major challenge for considering uncertainty in MFA. Consequently, the evaluation of the information basis for an MFA and the evaluation of data quality (first step in Figure 1) are the foundation of sound uncertainty analysis in MFA (cf. Schwab 2016). In the present study the concept of information defects was introduced to express the quality (or deficiency) of MFA data as a function of data characteristics. Thus, data quality is treated as a multidimensional problem that is assessed in view of various characteristics (see Schwab et al. 2017), which serve to express the degree of imperfection. Information defects are determined along four dimensions (semantics, representativeness, provenance, and context) and finally aggregated to the total information defect (ID_{tot}). The whole procedure of quantifying information defects was illustrated via a case study on palladium flows in Austria and compared to the uncertainty characterization in the original study (see *[4]*). On the one hand, it confirmed the practicality of the presented approach, on the other hand, it showed that the information defects (scale between 0 and 1) of individual flows were compatible with the uncertainty estimates (expressed as relative standard deviations) determined in the original study. However, implementing extensive data quality assessment procedures in MFA requires additional effort, which could be facilitated by a general system structure and standardized data formats for regional MFA studies (cf. Pauliuk et al. 2015).

The major contribution of this study to uncertainty analysis in MFA lies in the evaluation of the degree of credibility of MFA input data prior to the (mathematical) characterization of uncertainty and before the data is processed in the model. Although data quality assessment is and will remain inevitably subjective, investing a little more resources into an MFA by applying the procedures presented in this study enables transparent and consistent documentation, characterization, evaluation, and communication of the MFA information basis. The generation of uncertainty estimates to be used in material flow modeling (subsequent step in Figure 1) based on such an evaluation of the information basis,

provides a maximum of transparency about the use and reliability of information to quantify the material flow system.

2.1.3 A novel approach for characterizing data uncertainty in MFA (*Publication [3]*)

An approach to characterize the uncertainty of MFA input data was developed and applied to a case study on plastics flows in Austrian consumption sectors in *[3]*. The uncertainty characterization approach consists of three steps and builds on the existing pedigree matrix for life cycle inventory data by Weidema and Wesnæs (1996) (first step) and the data classification scheme by Hedbrant and Sörme (2001) (second step). In the first step of the approach, data quality was assessed using five data quality indicators (reliability, completeness, temporal correlation, geographical correlation, and other correlation). Evaluation criteria were defined to assign scores between 1 (very good fit) and 4 (poor fit) for each indicator. In the second step, the scores were transformed into quantitative uncertainty estimates using continuous functions (following either a linear- or exponential mathematical relationship). In the final step, the uncertainties due to imperfection along the five data quality indicators were aggregated to the total uncertainty of the MFA input data and the a priori[1] uncertainty estimates for the material flows are determined. With respect to the uncertainty characterization two different probability distributions (normal vs. log-normal distribution) were considered as alternatives and the effect on the case study results was analyzed. The case study showed that the choice of normal vs. log-normal distribution to express uncertainty had a relatively smaller effect on the uncertainty of the plastics flows than the use of exponential- vs. linear-type functions to link uncertainty estimates to the various data quality indicator scores. However, in case of highly uncertain flows (coefficient of variance >50%), the differences between the normal vs. log-normal distribution implementations were more significant. In addition, the definition of log-normally distributed material flow variables restricts the range of values to positive numbers, which is the case for physical material flow data. Whereas the restriction to positive values only is an advantage of the log-normal distribution, the generally easy handling and the implementation of the normal distribution assumption in the widely used STAN software for MFA (cf. Cencic and Rechberger 2008) are advantages of the normal distribution implementation. In any case, the lack of empirical data requires subjective choices during data uncertainty characterization, which puts the focus on consistent uncertainty estimates within a specific MFA study rather than on the comparability of uncertainty estimates between different studies (see [7] on this topic).

The major achievement of this work was to develop and apply a methodology for uncertainty characterization (initial step in Figure 1) tailor-made for MFA. Compared to the data quality assessment framework in *[2]*, the presented approach is less resource intensive and it

[1] A priori is used here to highlight that the uncertainty of material flow results may be different from the input uncertainty of the flows due to error propagation and data reconciliation procedures.

directly links data quality and uncertainty of material flow model inputs. Thus, it is directly related to established MFA practice. Since its development, the approach has already been implemented in several MFA studies (e.g. Buchner et al. 2014, Van Eygen et al. 2017, Zoboli et al. 2016a).

2.1.4 Uncertainty in MFA using fuzzy set and probability theory (*Publication [4]*)

In this study, the focus lay on the implementation of two fundamentally different uncertainty representation concepts and their effect on MFA outcomes, illustrated via a case study on palladium flows in Austria. After initial data quality assessment, two different mathematical frameworks were used to characterize uncertainty. In one case, uncertainty ranges were expressed as normal distributions given by mean value and standard deviation (cf. Figure 3). In the other case, uncertain variables were defined as fuzzy numbers via membership functions of trapezoidal or triangular shape. The former resembled the traditional quantification of uncertainty in MFA (cf. Baccini and Bader 1996), which was also implemented in the STAN software (http://www.stan2web.net/). The latter had hardly been used in the context of MFA (Dubois et al. 2014, Guyonnet 2012), but held the promise of being well suited for expressing imprecise or incomplete information (cf. Clavreul et al. 2013) and, therefore, increase the reliability of MFA results in situations of poor data or scarce information. For normally distributed uncertain variables, the procedures for data reconciliation and error propagation established in the STAN software were used to derive the material flow results (cf. Cencic 2016). For fuzzy sets, mathematical operations were performed according to the extension principle (cf. Viertl 2011) and reconciliation was done using a linear optimization algorithm (Tan et al. 2008).

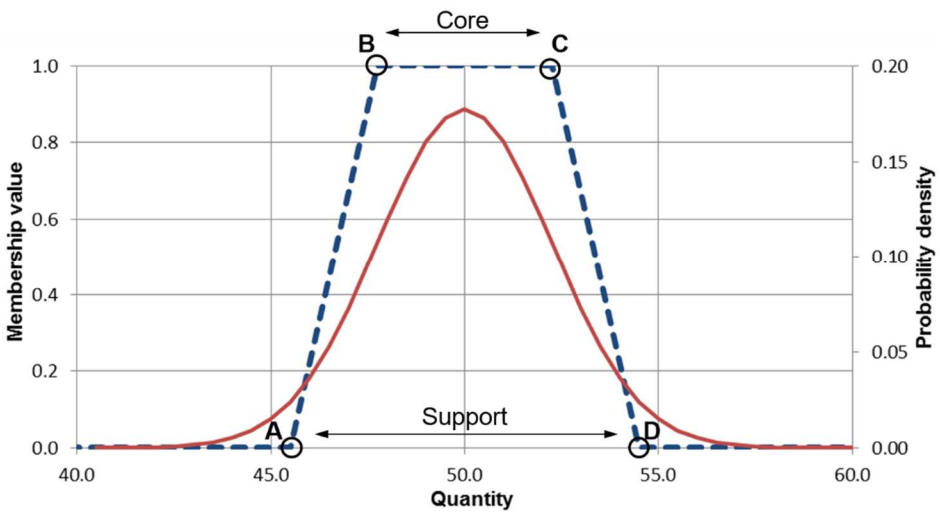

Figure 3: Illustration of a variable defined by a normal probability density function (mean value= 50, standard deviation= 2.25) and by its equivalent trapezoidal membership function (fuzzy set: base [A= 45.5, D= 54.5], core [B= 47.25, C= 52.25])

In general, the fuzzy set implementation resulted in wider uncertainty ranges, compared to the 95% confidence intervals of the normal implementation in STAN. In the case of fractional or incomplete data, the fuzzy set implementation was better suited to capture the effect of data limitations on the resulting material flows. Hence, fuzzy sets provided a suitable means for formally expressing the need for additional data to improve the understanding of anthropogenic resource systems, which is seen as a crucial issue with respect to many critical raw materials (cf. RPA 2012). For both, the “normal” and the “fuzzy” approach, data reconciliation enabled a reduction of flow uncertainties and plausibility checks of the model outcomes, highlighting the potential of data reconciliation procedures to indicate the quality of material flow analysis results.

This study was the first to compare the traditional “normal” approach of uncertainty representation in MFA to an approach building on fuzzy set theory using a full-scale MFA on palladium as a case study. Apart from demonstrating the implementation of two fundamentally different uncertainty concepts (first and second step in Figure 1), this work showed that the fuzzy approach is particularly well suited to express the effect of incomplete or poor-quality data on the uncertainty of MFA results (see *[5]* for a follow-up study). Independent of the uncertainty concept applied, it was shown that the generation of independent estimates for as many material flows as possible is essential to evaluate the plausibility of MFA results based on the analysis of data reconciliation procedures.

2.1.5 A fuzzy set-based approach to data reconciliation in MFA (*Publication [5]*)

In this study, a generally applicable method for data reconciliation under fuzzy constraints was developed and applied to a case study on wood flows in Austria. For each material flow, the reconciliation procedure resulted in a reconciled range of possible values (support = possible range, core = most likely range) and a level of consistency (= α), which indicated the agreement between given input data and the mass balance constraints of the model. The results were illustrated via Sankey-style diagrams, where the flow thickness was equivalent to the average flow value (calculated as mean of the core values, cf. Figure 3) and the flow color indicated the level of consistency.
A graphical example of reconciling two triangular membership functions is shown in Figure 4, for two cases with different ranges and different consistency levels (a: value between 4 and 6, α= 0.39; b: value between 2 and 8, α= 0.67). This example highlights an important finding of the study: There is a trade-off between the confidence in the data (i.e. the higher the confidence, the narrower the intervals) and the resulting flow consistency levels. Consequently, the consistency levels provide a quantitative measure to assess MFA results, because poor agreement in the model (= low consistency) does not justify high confidence in the data and vice versa.

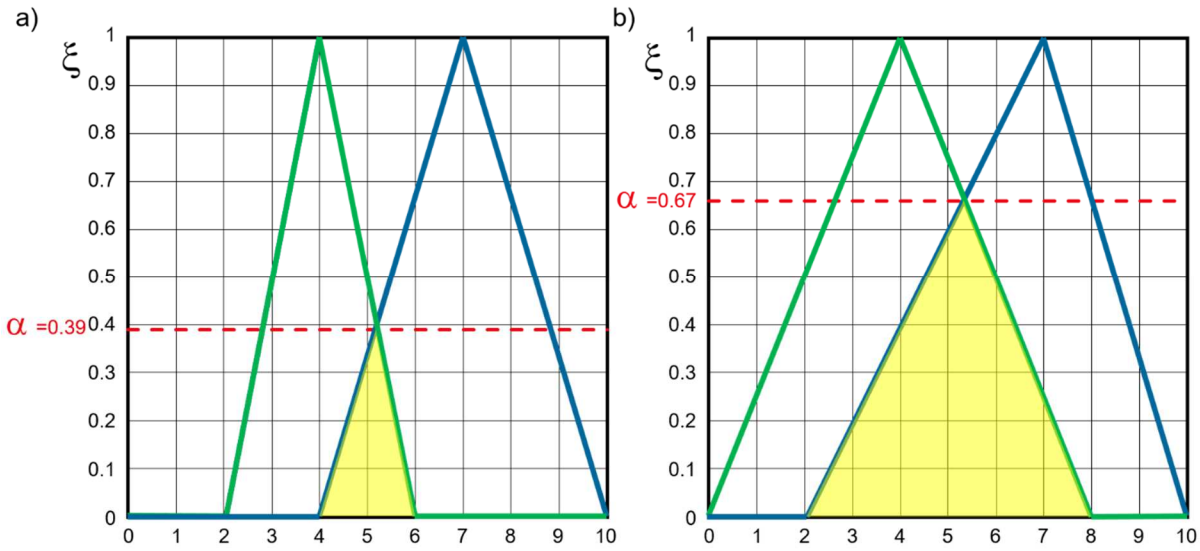

Figure 4: *Reconciled membership function (yellow shaded area) for two cases of two given triangular membership functions (based on [5]): a) poor agreement (low α), b) better agreement (higher α).*

A major innovation of the developed method compared to existing fuzzy reconciliation methods such as the leximin approach (Dubois et al. 2014) or fuzzy linear programming (cf. Tan et al. 2007) was that it could handle any kind of membership function and is not restricted to linear-type functions. Therefore, it offered maximum flexibility concerning the derivation of membership functions from the data quality assessment and provided consistent procedures to reconcile the input membership functions given the mass balance constraints of the model (step 2 in Figure 1). In view of material flow analysis being an iterative procedure, an important utility of the developed method was the identification of problematic data and model weaknesses as a basis for increasing the reliability of MFA results. Furthermore, methods for illustrating and exploring the relationships between consistency of and confidence in material flow results (step 3 in Figure 1) were also put forward in this work.

2.1.6 Sensitivity analysis in dynamic MFA (*Publication [6]*)

In this work, the focus was on analyzing the effect of input or parameter uncertainty on the uncertainty of dynamic material flow models. An archetypical top-down dynamic model (cf. Laner and Rechberger 2016) based on a dynamic MFA for aluminium (cf. *[8]* and *[9]*) was established and global sensitivity analysis (cf. Saltelli et al. 2008) were performed for different model settings. The variance of the model output was decomposed into fractions caused by the uncertainty or variability of input parameters (i.e. sector-specific product lifetimes, sector-split ratios). Interaction and time-delay effects of uncertain parameters on the model output were investigated to derive recommendations on the use of different sensitivity analysis methods (i.e. one-at-a time method, algorithms based on Fourier transformations (cf. Plischke 2010), variance-based sensitivity analysis) in case of different

model set-ups. The analyses showed that in classical dynamic models interaction effects between parameters were of minor importance for the sensitivity of the results. In general, end-of-life flows were more sensitive to variations in average lifetimes during periods of changing output, whereas variations in sector split had a dominant effect on end-of-life flows during periods of stable output. In case of time-dependent parameters, parameters in each period of change should be treated as separate variables in order to capture potential time delay effects. However, because dynamic material flow models are expected to become more complex in the future due to the introduction of closed mass balances (recycled material flows need to match the quantities used in secondary production, e.g. Nakamura et al. 2014), interaction effects may become more relevant in such set-ups. Finally, to account for varying model structures and purposes of dynamic MFA, a decision scheme for selecting appropriate sensitivity analysis methods in dynamic MFA studies was presented.

The major achievement of this study lay in the investigation of interaction and time-delay effects of parameter variation on the output of dynamic material flow models. Whereas sensitivity analysis in dynamic MFA was previously based on one-at-a-time methods, the present study used variance-based global sensitivity analysis to decompose the variance of the model output into fractions caused by parameter variation. The recommendations on appropriate sensitivity practices in dynamic MFA developed in this work facilitate the identification of critical input data as well as the interpretation and communication of dynamic MFA results in view of parameter uncertainty (step 3 in Figure 1).

2.1.7 Effect of data structure and model choices on MFA results (*Publication [7]*)

The goal of this study was to show how choices in national material flow analyses, i.e. characteristics of the material flow model not directly resulting from the physical properties of the systems studied, influence the results. Therefore, two recent phosphorus balances for Austria (Zoboli et al. 2016a) and Denmark (Klinglmair et al. 2015) were compared with respect to their system boundaries, model structure, input data, and uncertainty assessment. Whereas the differences in the system layouts were attributable to deviating goal and scope definitions of the studies, significant differences in the uncertainty assessments existed despite relatively similar data availability and types of data sources. The reconciliation of conflicting flow data was analyzed for both studies by comparing the input data to the reconciled values. It provided a meaningful measure for the consistency of input data given the mass balances in the models. Overall, the Austrian balance was slightly more consistent than the Danish balance, because the average change between input flow data and reconciled flow values was 5% compared to 9 % in the Danish case. Hence, although a direct comparison of uncertainty ranges between different studies appeared to be problematic due to subjectivity inherent in the uncertainty assessment, the comparison of consistency measures based on data reconciliation procedures could provide an indication of model quality across MFA studies. This highlighted the need for transparent procedures concerning system definition and uncertainty characterization in MFA (step 1 in

Figure 1) to allow for direct and consistent comparisons between key material flows and efficiency indices, such as collection or recycling rates (cf. Haupt et al. 2017).

The major advancement in this study was the investigation of model and scenario uncertainty related to country-level MFA studies. So far, uncertainty analysis in MFA had mainly been concerned with parameter uncertainty and little research had been done on understanding the effect of modeler's choices on the outcome of MFAs. Based on the comparison of the phosphorus budgets for Austria and Denmark, a generally applicable approach to analyze and transparently document choices in MFA was outlined. Therefore, the outcomes of *[7]* enabled robust interpretation of MFA results within a specific study and facilitated analyses across different MFA studies.

2.2 Analysis of resource system dynamics

Dynamic material flow analysis (dMFA) is used to investigate resource utilization patterns over time, material stock build-up in society, as well as the development of emission levels related to changes in production, consumption, and waste management (cf. Laner and Rechberger 2016). Thus, dMFA provides information about material use over time and consequent changes in stocks and flows within the system. Whereas material flows in a static MFA are time independent (i.e. snapshot of the resource system), material flows in a dynamic model may depend on all previous states of the system (cf. Baccini and Bader 1996). In the past, most MFA studies used static models to investigate material flow systems, but during the last three decades the use of dynamic models to investigate material resource systems has increased tremendously (cf. Chen and Graedel 2012a). Metals, in particular, have been subject to dynamic MFA due to the large accumulated metal stocks in society and their potential value for society as secondary raw materials (cf. Müller et al. 2014). In most dynamic MFA studies, a delay model is used to determine the material output from the stock based on the convolution of (discretized) lifetime distributions and the material input to the stock (e.g. in-use phase) over time. The material output contained in a specific product i in period T, $m_{O,i}(T)$, is calculated by the numerical solution of Equation 1, where $m_{I,i}(T - d)$ is the material input in product i d periods before T and f(d) is the discretized probability density of the lifetime distribution function for d. A frequently used lifetime function in dMFA from the field of system reliability is the Weibull distribution (cf. Müller et al. 2014). Apart from that, also normal, log-normal, beta, and gamma distributions are used in dMFA to consider the residence time of materials in use (cf. Melo 1999). The total material output in period T, $m_{O,i}(T)$, is the sum over the k different products considered in the model (see Equation 2). The total material stock in period T, S(T) can then be derived by considering the initial stock, S(0) and summing up the stock changes (i.e. material input – material output) for all previous periods (see Equation 3). The method to determine the material stock S at the time T described in Equations 1-3 is termed "top-down approach" and is most frequently used in the field of dynamic material flow analysis to investigate the

evolution of material stocks (cf. Müller et al. 2014). The alternative method to determine the stock at a certain time is called “bottom-up approach” and is based on summing up the material contents of all relevant products in stock at the time of interest (e.g. Tanikawa et al. 2015).

$$m_{O,i}(T) = \sum_{d=0}^{T} m_{I,i}(T-d) \cdot f(d) \qquad \text{(Equation 1)}$$

$$m_O(T) = \sum_{i=1}^{k} m_{O,i}(T) \qquad \text{(Equation 2)}$$

$$S(T) = S(0) + \sum_{d=0}^{T} m_I(T-d) - m_O(T-d) \qquad \text{(Equation 3)}$$

The combination of the bottom-up and top-down methods to calibrate and validate a dynamic material flow model is illustrated in *[8]* for the case of aluminium (Al) resource use in Austria. Because dynamic models are usually more complex and have a higher data-demand than snapshot MFAs, calibration of model parameters and extensive plausibility checking of model results is crucial for obtaining reliable MFA results. The calibrated and validated model can subsequently be used to analyze trends in material use over time and to forecast future system behavior based on scenarios. This was done in *[9]* to evaluate the development of future Al stocks in different sectors in Austria and to anticipate the future availability of Al scrap. However, like most other existing MFA studies (e.g. Chen and Graedel 2012b, Liu and Müller 2013), aspects of material quality (e.g. alloy composition) and their effect on secondary raw material utilization have not been addressed in *[9]*. Therefore, the existing Al model was expanded in *[11]* to consider different Al alloys (wrought and cast) and assess potential limitations for Al recycling due to inappropriate alloy mixtures in Al scraps. Another study which considered the quality of end-of-life (EOL) material flows was reported in *[10]*, where the future contamination of EOL wood from buildings was evaluated using dynamic material flow modeling. Furthermore, in *[10] the* case study on wood from Viennese buildings was also used to compare different modeling approaches (delay vs. leaching model) and identify situations when one or the other approach may be appropriate to estimate EOL material flows from buildings. Because buildings constitute the largest material stock of our society and the amount of construction & demolition waste (CDW) has been increasing continuously in the past (and will in the future), appropriate methods to forecast the quantity and quality of EOL material flows from buildings are essential for exploiting the resource potential of the built environment (cf. Augiseau and Barles 2017).

In the light of efforts to further enhance the circularity of product systems (e.g. EC 2015), dynamic MFA can be used to track recycled materials, especially on the substance level, during subsequent product cycles. Except for a few notable examples (cf. Nakamura et al.

2014, Nakamura et al. 2017, Pauliuk et al. 2017), the quantity and quality of the material directed to recycling is typically not preserved in the production process of the next cycle in dMFA. However, this is a vital model characteristic to investigate the role of problematic contaminants in secondary production systems and identify trade-offs between the quality and quantity of secondary raw materials. Against this background, *[12]* aimed at the quantitative evaluation of the cycling of problematic substances and subsequent product contamination via a consistent modeling approach applied to chemicals flows in the European paper cycle. Based on these pioneering works, closed balances on the goods and substance levels are expected to become a key feature of dynamic material models to analyze and evaluate the transition towards a circular economy.

2.2.1 Aluminum stocks and flows in Austria 1964 – 2012 (*Publication [8]*)

The present study aimed at developing a calibrated and validated dynamic model of Austrian aluminium (Al) flows from 1964 to 2012 to determine the evolution of in-use stocks and end-of-life (EOL) flows. Although dynamic MFA studies on Al existed on the international and national levels (e.g. Chen and Graedel 2012b, Ciacci et al. 2013, Cullen and Allwood 2013, Müller et al. 2014), data-based model validation as well as uncertainty and sensitivity analysis were typically not dealt with in these studies. Therefore, a particular focus of this work, apart from rigorous uncertainty and sensitivity analysis, was on contrasting the results of the top-down dynamic model with bottom-up estimates (based on independent data sources) as a basis for cross checking and validating the model estimates. Independent (bottom-up) data were available also for the annual Al input into the transport sector and the packaging sector to calibrate the model. Although calibration was only possible for these two out of the six in-use sectors, the results showed that literature data on the consumption share of different sectors deviated strongly from actual country-specific parameter values and that Al consumption patterns (sector shares) varied substantially over time, indicating the use of constant parameter values in many dynamic MFA studies to be problematic. The validated model results showed that the total Austrian in-use Al stock was around 360 kg per capita in 2012 (nearly half in the building and construction sector and one third in the transport sector) and that EOL Al flows (12 kg/cap and yr) amounted to approximately half of final Al consumption (25 kg/ca and yr). The model results generated a detailed understanding of the evolution of Al stocks and flows in Austria, providing a reliable basis for evaluating recycling potentials and developing Al resource management strategies on the national level.

The major contribution of this study lay in contrasting top-down model parameter estimates and results with independent bottom-up data as a basis to calibrate, cross check and validate dynamic material flow models. Furthermore, uncertainty and sensitivity analyses were carried out to evaluate the reliability of model outcomes and identify factors and assumptions strongly affecting the model results, which highlighted that there is a lack of

sensitivity analysis procedures considering parameter interaction as well as time-delay effects in dynamic MFA (this work was carried on in study *[6]*). Finally, the focus on the national level enabled data-based model evaluation and improvement, because such information is typically available for individual countries due to specific (and internationally not standardized) data collection and reporting schemes. Hence, the outcomes of this study constituted a sound basis for establishing scenario-based predictions of future Al stock development and consequent scrap availabilities (see *[9]*) and, therefore, for optimizing the management of anthropogenic Al resources.

2.2.2 Future aluminium raw material supply from end-of-life flows (*Publication [9]*)

This study combined a dynamic material flow model of historic aluminium flows in Austria (cf. *[8]*) with scenarios about future Al consumption to estimate the development of national old scrap generation and in-use stocks until 2050 (see Figure 5). The current (2012) Al in-use stock was determined using the historic model for the different use sectors. For some of these sectors (Transport, Buildings & infrastructure, Electrical engineering), predictions on the future development of the stock were established based on demographical, societal and technological trends to determine future Al input flows (=stock-driven approach). For the other sectors (Mechanical engineering, Consumer products, Packaging) estimates on specific annual growth rates of final consumption were used to determine future Al consumption (=input-driven approach). Three different scenarios were analyzed to cover a range of possible developments, (low, middle, and high Al consumption, respectively). Assuming moderate growth of Al consumption levels (=middle scenario), in-use stocks were estimated to increase by more than half from 2012 (360 kg/cap) to 2050 (515 kg/cap). Furthermore, old scrap generation was expected to increase more than two-fold until 2050 to 30 kg/cap and year. This increase in the availability of EOL Al was confronted with the Al demand to satisfy i) final Al consumption in Austria (=potential final consumption self-supply) and ii) raw material demand of the (highly export-oriented) Austrian Al industry (=potential industrial self-supply) to evaluate the potential for Al self-supply. The evaluation showed that Al self-supply (in a hypothetically closed system) would not exceed 20% in terms of industrial-self supply and 40% in terms of final consumption-self supply. Even the termination of EOL vehicle exports and enhanced Al recycling from wastes could not raise the potential final consumption self-supply level above 74% in 2050. Hence, full domestic supply of Al from EOL flows could not be reached without a decrease in consumption levels, despite the expected growth in scrap quantities. This statement was exacerbated by the fact that increasing self-supply via old scrap may result in unsuitable Al alloy compositions for remelting. The mix of various alloys in Al scrap flows could be a limiting constraint for the amount of old scrap utilizable in secondary production. Therefore, the compatibility between future Al scrap qualities and Al raw material demand in secondary production was investigated in *[11]*.

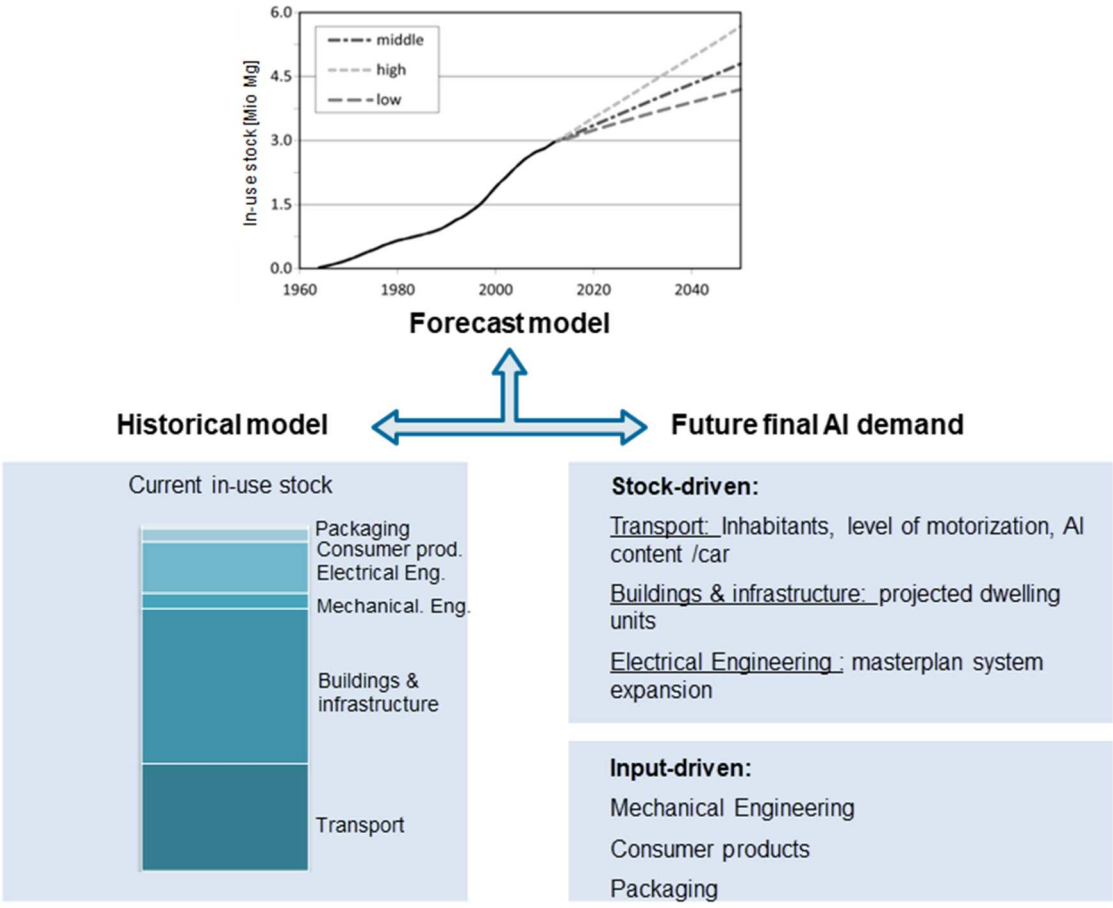

Figure 5: Schematic illustration of the model framework to predict future stocks and flows of Al in Austria

By analyzing future trends in potential old scrap generation and in-use stock development for Austria, two major contributions to the understanding and management of anthropogenic Al resources were made by the present study. First, scenario-based estimates for the future development of Al in-use stocks and EOL flows (=old scrap generation) were provided and, together with the analysis of historical Al use patterns (see *[8]*), enabled a profound understanding of anthropogenic Al resource potentials and their dynamics. Second, the potential of Al scrap to satisfy domestic Al raw material demand was evaluated from a quantitative perspective, highlighting that a fully circular Al resource system (without the need for external Al raw material input) could not be expected (until 2050) despite increasing scrap generation rates and despite neglecting alloy-specific constraints in secondary production.

2.2.3 Modeling end-of-life wood flows from Viennese buildings (*Publication [10]*)

The objective of this study was to evaluate different modeling approaches to predict the quantity and quality of end-of-life building material flows. Wood in Viennese buildings was used as a case study. Two archetypical modeling approaches were identified (delay approach based on lifetime functions vs. leaching approach based on a leaching share of the stock) and implemented to determine EOL wood flows from buildings in Vienna and the flows of major contaminants (lead - Pb, chlorine - Cl, polycyclic aromatic hydrocarbons - PAHs) potentially constraining wood recycling. In accordance with previous studies (cf. Kleijn et al. 2000, van der Voet et al. 2002), it was found that the delay approach was better suited to investigate the effect of historic wood use in buildings on current stocks and EOL flows as well as to determine the contamination levels with respect to specific substances in EOL wood flows. However, for the estimation of future wood flows related to buildings in Vienna, the (per definition) limited lifetime of, in particular, old (>100 years) buildings turned out to be a shortcoming of the delay approach (due to the persistent share of historical buildings in stock). Thus, although the modeling of age cohorts of buildings (i.e. delay approach) turned out to be superior to assuming a share of the material stock to become obsolete (i.e. leaching approach), it should be adapted to account for “immortal buildings”, which are not demolished but constantly maintained. Apart from the methodological findings, the study showed that the amount of EOL wood from Viennese buildings is not expected to increase in the future (like in the past), but may remain rather constant or decrease slightly. The contamination levels of Pb, Cl, and PAHs are on the decrease due to the ban of many applications of these substances in the past, but they are expected to be of relevance as legacy contaminants in recycling wood also during the coming decades.

The present work made a significant contribution to the investigation of the building stock as a source for secondary raw materials concerning methods as well as application. On the one hand, the comparison and evaluation of modeling approaches, including an extensive review of dynamic MFA studies on C&D (construction & demolition and renovation) waste, provided a basis for implementing appropriate modeling techniques specific to the objectives of an MFA study. On the other hand, the determination of EOL wood flows from Viennese buildings and their respective contamination with substances critical for wood recycling constituted the basis for assessing the wood resource potential of the Viennese building stock in terms of quantity and quality.

2.2.4 A closed Al system: recycling constraints due to scrap quality (*Publication [11]*)

The goal of this study was to investigate future Al scrap generation and utilization in Austria considering different alloys (i.e. wrought vs. cast alloys) with respect to the potential for a closed Al cycle. Therefore, an existing dynamic material flow model ([9]) of Austrian Al flows between 1964 and 2050 was expanded to consider wrought and cast Al alloys. Furthermore, a closed system was assumed where all the domestic Al scrap supply was

used to satisfy the Al demand associated with domestic final consumption. The results showed, that a surplus of cast and mixed Al scrap over cast Al demand could be expected, if wrought and cast alloys in mixed Al scraps (especially from the transport sector) are not separated in the future. Given the expected increase of wrought Al usage in cars, a situation of domestic over supply due to inadequate scrap quality may already occur in 2030. Apart from intensive sorting, international scrap trade was found to be a key element for bridging the gap between domestic scrap supply and the scrap demand for secondary production.

This study closed an important research gap related to investigating the potential for closed material cycles on the regional or national level by investigating the future supply and demand for Al scrap in Austria from a quantity and quality perspective. Before, only few MFA dynamic MFA studies had addressed alloy compositions of Al scraps (e.g. Cullen and Allwood 2013, Hatayama et al. 2007) or had a focus on Al alloys in specific sectors (e.g. Løvik et al. 2014, Modaresi and Müller 2012) and none of them evaluated the potential for closing regional material cycles. Therefore, the present study was the first to show that material quality aspects will become more and more critical for the utilization of Al scraps as secondary raw materials during the coming decades and that enhanced sorting as well as international scrap trade are suitable strategies for mitigating quality constraints on the national or regional level. Thus, old scrap processing in terms of alloy sorting may become a key element of strategies to achieve more circular resource use on the regional level.

2.2.5 Chemicals flows in the European paper product cycle (*Publication [12]*)

The goal of this study was to develop a systematic approach for investigating contaminant cycles in secondary production systems and illustrate its use to assess flows of selected chemicals (bisphenol A - BPA, diethylhexyl phthalate - DEHP, mineral oil hydrocarbons – MOHs) in the European paper cycle. The developed approach combined static and dynamic material flow modeling (see Figure 6). First, the current (year 2012) use pattern for paper products in Europe was analyzed in a static MFA. In the second step, the amount of chemicals added to the cycle per year as well as the level of contaminant cycling in paper products based on waste paper analyses and assumptions on chemicals partitioning during production, conversion and use was determined. The transfer coefficients derived from the material and substance balances were then used to set up a dynamic material flow model, which served to investigate the effect of different mitigation measures (i. optimized waste paper collection, ii. intensified chemicals removal during production, iii. ban of chemicals use in products) on the contamination levels in paper products (3. in Figure 6). Although the data on substance use in products was very limited and many assumptions had to be made (e.g. identical chemicals concentrations in domestic and foreign trade flows, substance removal efficiencies during production based on equilibrium models, etc.), it was possible to identify chemicals phase out (iii.) as the most effective strategy to mitigate chemical contamination of paper products and optimized waste paper collection (i.) as the least effective one. The latter was true, if paper collection rates were to be maintained on the

current levels (on average 70% in Europe). However, if lower (mass-based) collection rates were acceptable (which is against the general trend in paper recycling, however), significantly lower chemicals flows into secondary production could be achieved by optimized waste paper collection. Hence, the results of this study highlight that material recycling needs to be a balance between high quality secondary raw materials and high (mass-based) recycling levels.

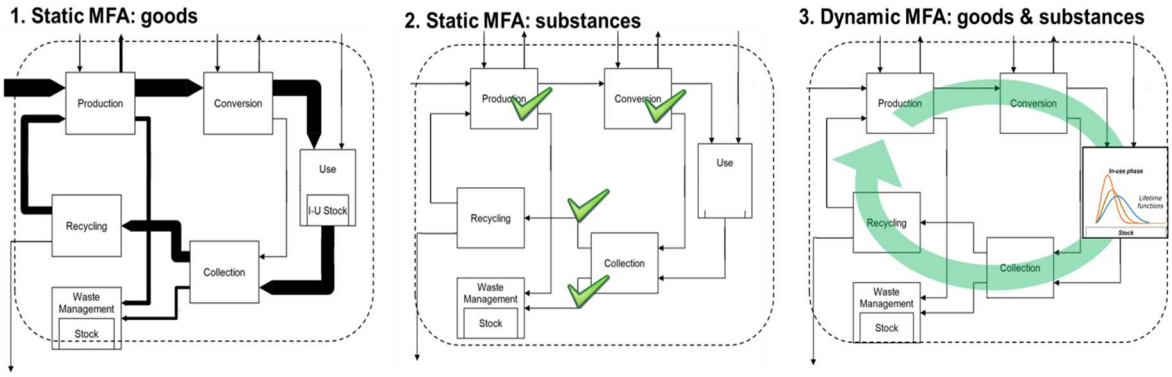

Figure 6 : Modeling approach to investigate chemicals flows in a product cycle based on the combination of static and dynamic MFA (adapted from [12])

One major achievement of this work is the provision of a systematic approach for assessing chemicals contamination of product cycles from a material flow perspective. Although the issue of clean cycles and appropriate sinks for problematic substances has been identified as an important field of research (Brunner 2010, Brunner and Tjell 2012, Kral et al. 2013), this is the first study to quantitatively evaluate the cycling of problematic substances and subsequent product contamination via a consistent modeling approach and a concrete case study. Given the importance of clean material cycles and the challenge of directing problematic substances to appropriate sinks, the presented modeling approach should be further developed and also applied to other product cycles and chemicals in the future (e.g. cascading use of wood or plastics recycling). Furthermore, a link between recycling and human exposure to chemicals in secondary products could be established building on the presented approach, which constitutes the basis for assessing the risks of chemical contamination in material cycles. Hence, the explicit consideration of substance flows in material cycles represents a key tool for investigating the environmental performance of increasingly circular product systems.

2.3 Evaluation of resource recovery strategies

Material flow analysis is fundamental to the understanding of resource utilization in an economy and provides the basis for investigating resource use at a certain time. From a waste system's perspective, MFA can be used to assess the safe handling and disposal of hazardous substances and the recovery of valuable resources from wastes (cf. Allesch and

Brunner 2017, Brunner and Rechberger 2016). The balancing of flows on the goods and substance levels in a material flow model generates inventory data for waste management processes and process chains, which are required to assess resource efficiency or environmental performance as a basis to choose environmentally optimal waste management solutions (e.g. Tonini et al. 2013, Vadenbo et al. 2014). Thus, to communicate MFA results unambiguously and to link material flows to environmental impacts or resource depletion issues, evaluation is an essential step on top of MFA studies (cf. Allesch and Brunner 2015).

Detailed plant-level or technology-level MFAs have been used in waste LCA studies to investigate substance and energy flows of new treatment technologies and to evaluate their environmental performance compared to other waste treatment alternatives. In *[13]* material and energy flow analyses of different technologies for treating end-of-life (EOL) cooling appliances were combined with life cycle impact assessment (LCIA) indicators to assess the influence of increasing recycling levels on the environmental performance of EOL cooling appliance management. Also in *[14],* MFA and LCA were combined to identify environmentally optimal waste treatment technologies for handling municipal solid waste incineration (MSWI) fly ash. The climate impact of landfill mining as a resource recovery strategy was in the focus of *[15]*, where a generic scenario modeling approach was developed to assess a landfill mining project's contribution to global warming based on material (goods level and carbon) and energy balances, life cycle inventory databases and life cycle impact assessment. Therefore, the above studies (*[13]*, *[14]*, *[15]*) assessed the environmental performance of resource recovery from different waste types as a basis for identifying optimal solutions or strategies on the technology level. Similarly, evaluations of whole waste systems can be performed building on a combination of MFA and LCA. From a systems perspective, resource quality aspects are of particular importance in addition to the consideration of mass flows, because the utility of a specific material flow is closely related to its composition, the utilization pathways within the resource system, and the interaction with other resource systems. The resource efficiency of resource recovery from residual household waste was assessed using exergy analysis in *[16]*, where resource quality was expressed via exergy content or cumulative exergy required to provide a product or service. Exergy does not satisfy a law of conservation and the idea is that exergy destruction should be minimized throughout the processes of resource use (cf. Ayres et al. 1998, Ignatenko et al. 2007, Szargut 2005) in order to keep functionality high. However, with respect to macro-scale MFA, the calculation of flow exergies is impractical as information on the detailed composition (chemical compounds) and physical state is not available. Therefore, the concentration of a resource in a material flow was suggested as a proxy for resource quality and operationalized in statistical entropy analysis (SEA), which is a method to evaluate material flow systems with respect to their ability to concentrate or dilute a substance throughout its material life cycle (Rechberger and Brunner 2002, Rechberger and Graedel 2002). The existing SEA method was further developed in *[17]* to enable assessing the efficiency of resource use in complex material flow systems with multiple resource flows and recycling loops. Using P-resource use in Austria as a case

study, *[17]* showed that statistical entropy can provide a meaningful indication of resource efficiency of macro-scale material flow systems and a suitable basis for optimizing resource use.

2.3.1 Identifying optimal recycling rates for end-of-life cooling appliances (*Publication [13]*)

In this study, MFA was applied in conjunction with life cycle impact assessment (LCIA) to investigate the environmental performance of two different technologies for the recycling of EOL cooling appliances. The study was motivated by the introduction of a legally required minimum recycling rate of 75% for EOL cooling appliances (FMAFEW 2005). The goal was to find out whether the minimum recycling rate would lead to better treatment of cooling appliances with respect to resource recovery and environmental protection. Therefore, two treatment technologies for EOL cooling appliances, which achieved recycling rates between 80 to 90% (T1) and 50 to 60% (T2), respectively, were compared. The focus was put on the treatment of cooling appliances containing Chlorofluorocarbons (CFCs), where material flows were determined on the goods (i.e. mass) level and for selected substances (CFCs, CO_2, HF, and HCl). Together with energy balances, the material balances formed the basis to assess the environmental impact in terms of Global Warming Potential (GWP), Ozone Depletion Potential (ODP) and Acidification Potential (AP) as well as resource depletion in terms of Cumulative Energy Demand (CED).

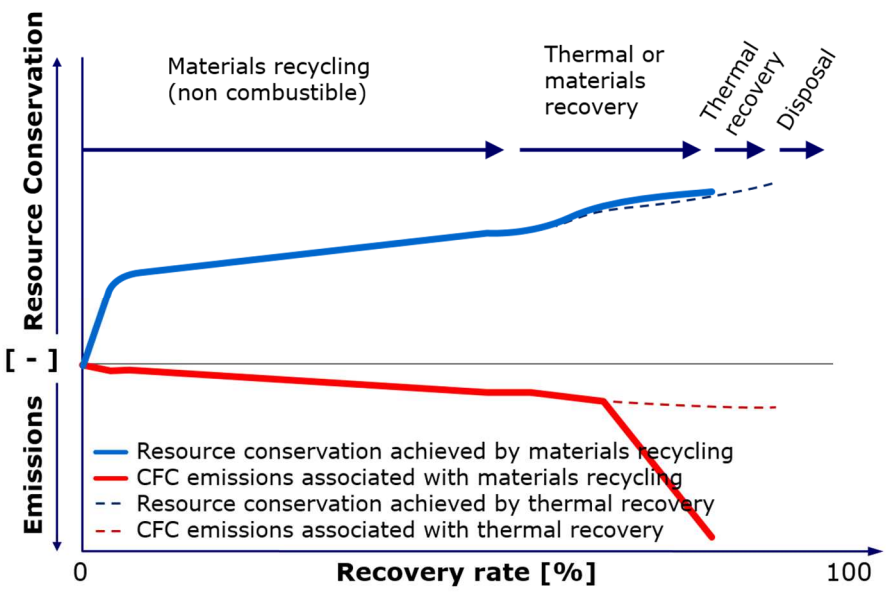

Figure 7: Emissions of CFCs and resource conservation (expressed as saving of cumulative energy demand) for the treatment of CFC cooling appliances using T1 (solid lines) and for a modified version of T1 with lower material recycling rates, where all plastics are incinerated (dotted lines) (based on [13])

The study showed that T1 achieved higher resource savings, but also resulted in higher ozone depletion, because of substantial CFC losses. The largest contribution to resource

conservation (CED) was achieved by the recycling of metals (aluminum, copper, and then iron) for both technologies. For T1, however, the material recycling of the polyurethane (PUR) insulation as an adhesive agent was associated with higher environmental impacts, because of dissipative emissions of CFCs from the PUR material (see Figure 7). An environmentally beneficial modification of T1 would therefore be not to recycle PUR, but to incinerate it at high temperatures with energy recovery (dotted lines in Figure 7). Although this would result in a lower average recycling rate for T1 (below 75%), it would achieve a similar level of resource conservation in terms of saving primary energy demand and result in significantly lower ozone depletion.

The major contribution of *[13]* was to find out whether or not the predefinition of minimum recycling rates is suited to achieve goal-oriented waste management solutions using EOL cooling appliances as a case study. Due to the popularity of legally pre-defined minimum recycling rates, the results of the study are relevant in many areas of waste management beyond the technical question of how to optimally recycle EOL cooling appliances. The study clearly illustrated that the optimal recycling rate is a function of waste composition and the technologies available for treatment and recycling. Furthermore, the raw materials substituted for by the waste-derived materials are central to evaluate the benefits of recycling, because the substitution of materials/products with a large ecological rucksack represents a higher potential for ecological savings than the substitution of less refined or readily available materials/products. Consequently, a high recycling rate alone does not ensure goal-oriented waste management.

2.3.2 Life cycle assessment of municipal solid waste incineration fly ash management options (*Publication [14]*)

The aim of this study was to compare five different scenarios for municipal solid waste incineration (MSWI) fly ash treatment and disposal using life cycle assessment (LCA). The management alternatives for MSWI fly ash (which is designated as hazardous waste) were a) deposition at underground deposits, b) deposition at above-ground landfills after cement stabilization, c) application of the FLUREC process, d) thermal treatment in a dedicated furnace, or e) thermal co-treatment together with combustible hazardous waste. The functional unit of the study was the treatment and disposal of 1 Mg of MSWI fly ash from a grate incinerator in Vienna. Material and energy flows were determined for all scenarios and emissions and resource consumption outside the respective waste treatment system were determined using life cycle inventory databases (i.e. ecoinvent V3.2) and literature data. The life cycle impact assessment was performed using the ReCiPe model by Goedkoop et al. (2009). The results showed that the FLUREC process (c) had the lowest environmental impact and that stabilization with cement (b) and thermal treatment in a separate furnace (d) performed worst from an environmental perspective. Whereas zinc recovery was environmentally beneficial (FLUREC process), it may only be economically feasible for MSWI fly ashes with exceptionally high zinc contents (cf. Fellner et al. 2015). In addition to

just comparing different MSWI fly ash management options, uncertainty analysis was used to investigate the effect of considering long-term emissions from the deposited residues (100 years vs. indefinite timeframe) for the ranking of the different scenarios. In the present case, it determined whether disposal at underground deposits (a) or thermal co-treatment with hazardous waste (e) were environmentally preferable over one another.

One major outcome of this work was the development of a life cycle assessment model for MSWI fly ash management, which can be adapted to different fly ash compositions and specific conditions. Thereby, it provides a tool for plant operators or waste owners to identify environmentally optimal management options for MSWI fly ash. Another important contribution of this study was the analysis of how the handling of long-term emissions in LCA affects the scenario rankings, which illustrates the significance of landfill models for the environmental performance of waste management (cf. Bakas et al. 2015, Hellweg 2000, Laner 2009).

2.3.3 Critical factors for the climate impact of landfill mining (*Publication [15]*)

This study aimed at evaluating major factors influencing the climate impact of landfill mining using a novel, set-based modeling approach to derive policy recommendations on facilitating the development of projects contributing to global warming mitigation. Whereas landfill mining has mainly been used to solve traditional waste management issues in the past (cf. Hogland et al. 2004, Krook et al. 2012), some recent projects have been initiated with the primary objective to recover resources for material recycling and energy recovery (cf. Jones et al. 2013, Van Passel et al. 2013, Winterstetter et al. 2015). In order to motivate political action to support such projects, it is central to understand their contribution to prioritized policy targets such as climate change mitigation. Because only case-specific assessments on the climate impact of landfill mining were available and because some of them resulted in net-saving of GHG emissions (e.g. Danthurebandara et al. 2015a, Frändegård et al. 2013) and others in net-burdens (e.g. Danthurebandara et al. 2015b, Winterstetter et al. 2015), a systemic understanding about which factors determine the climate impact of landfill mining was required to support sound policies and strategies for enhanced landfill mining. This was the goal of this study, which combined LCA, MFA, scenario modeling, and global sensitivity analysis to identify generic factors critical for the climate impact of landfill mining. First, eight major factors for the climate impact of landfill mining were identified based on existing studies (see Figure 8) and two or three alternative datasets were defined to reflect the typical range of parameter vales related to the individual factors. The alternative sets of the different factors were combined to 2916 scenarios and their net contribution to global warming was determined using an LCA model. The observed variation in the results was then decomposed to the contribution of individual factor variations using variance-based sensitivity analysis and with respect to individual parameter variation using step-wise linear regression modeling. The results showed that the global warming scores of the different scenarios ranged from net savings of -1.5 Mg CO_2e/Mg of

excavated waste to net burdens of 0.6 Mg CO_2e/Mg of excavated waste. Most of this variation could be explained by four factors, which are the landfill gas management in the reference case (i.e., alternative to mining the landfill), the background energy system, the composition of the excavated waste, and the applied waste-to-energy technology. Therefore, to maximally contribute to global warming mitigation, landfill mining should be implemented at landfills rich in organic waste with currently poor gas collection in regions with fossil-based energy systems and in the vicinity of highly efficient waste-to-energy plants. Based on the analyses in this study, tentative principles for facilitating projects contributing to reduced climate impacts could be outlined and policy-relevant knowledge to develop landfill mining strategies from a climate perspective could be provided.

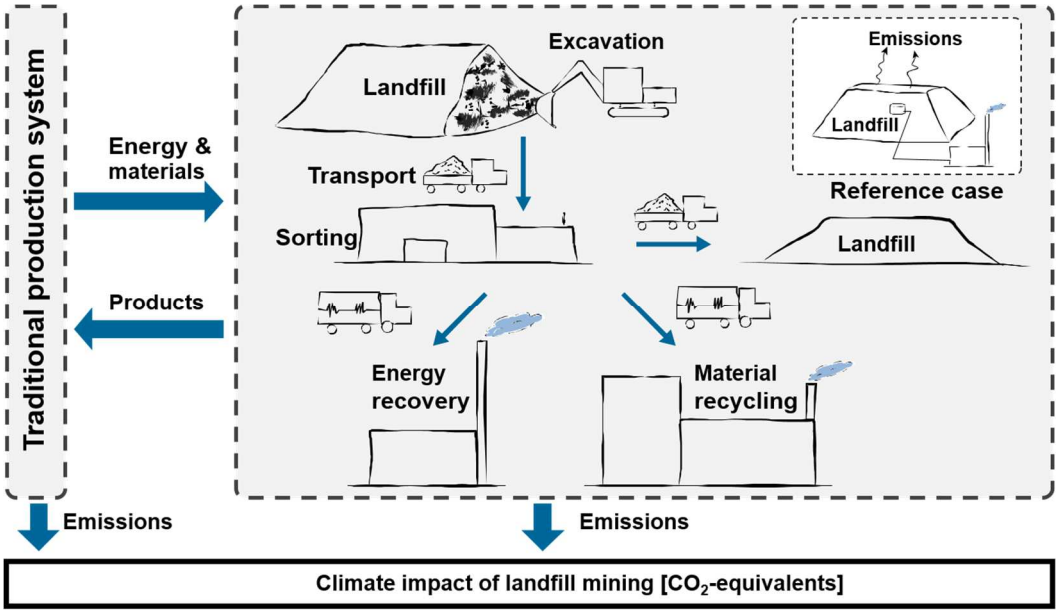

Figure 8: Schematic illustration of relevant factors for the climate impact of landfill mining projects (based on [15])

This study made two major contributions to the evaluation and implementation of landfill mining from the perspective of resource recovery and climate change mitigation: First, it is the first systematic analysis of the importance of different factors on the site, project, and system level for the climate impact of landfill mining. Based on the identification of critical conditions and circumstances, sound strategies and policies for facilitating climate-friendly landfill mining projects can be developed. Second, the analytical approaches and statistical methods developed in this study can be applied to different technology settings, where a systemic understanding on the role of specific factors and conditions for the environmental performance is to be established to support policy development and strategic planning. This broadens the relevance of this study from just landfill mining to diverse fields of waste and environmental management.

2.3.4 Exergy-based evaluation of resource recovery from household waste (*Publication [16]*)

Exergy has been put forward as a thermodynamically based (Second Law) measure for resource accounting (cf. Dewulf et al. 2008). This study aimed at giving recommendations for using exergy-based indicators to evaluate resource recovery from waste. Therefore, two exergy analysis methods were distinguished, which differed in the resource accounting method and the system definition. Exergy flow analysis mapped all the exergy flows and losses within the system under investigation. Exergetic life cycle assessment accounted for exergy flows following life cycle assessment (LCA) principles by applying the CEENE (= Cumulative Exergy Extraction from the Natural Environment) indicator (cf. Alvarenga et al. 2013, Dewulf et al. 2007) to the materials and energy consumed and produced by the system. The two approaches were applied to four scenarios, which involved increasing levels of source-segregation and recycling of selected resources (metals, plastics, and organic waste materials) from residual household waste. Detailed material and energy balances were established for each scenario and evaluated in terms of flow exergies or CEENE scores, respectively. The resource recovery efficiency was then determined for each scenario by dividing the flow exergies or CEENE scores of the useful outputs (= resource flows) by the flow exergies or CEENE scores of the consumed materials. Scenario efficiencies were low for both approaches, around 17–27% based on the exergy flow analysis (higher efficiencies were associated with high levels of material recycling) around 14% for all scenarios based on the exergectic LCA. Metal recovery was beneficial in both analyses, but contributed more to the overall efficiency in the exergetic LCA approach, due to the avoided burdens associated with primary metal production. Material recycling of plastics was highly beneficial in the exergy flow analysis, whereas in the exergetic LCA thermal utilization of plastics performed equal to material recycling. Thus, depending on the approach, different conclusions could be drawn regarding optimal resource recovery from residual household waste. However, the consideration of quality aspects was crucial for the obtained results in both approaches. In this respect, the major challenges for the exergy flow analysis were the use of exergy content and exergy losses as a proxy for resource quality and resource losses as well as the definition of appropriate waste system boundaries. For the exergetic LCA, resource quality was reflected by the savings achieved by product substitution, which involved several assumptions. Therefore, sensitivity analysis related to substitution choices are an essential element of comprehensive resource efficiency assessments in waste LCA.

The major achievement of the present study was the identification and evaluation of exergy-based approaches to assess resource efficiency of waste systems as a basis for optimizing resource recovery. Although each of the exergy analysis approaches is confronted with specific shortcomings, they can offer additional insights concerning strategies for resource recovery from waste. Exergy flow analysis maybe useful primarily for plant-level studies, because the use of exergy as a proxy for resource quality appears to be problematic in

larger systems with various material and energetic utilization options. Exergetic LCA is better suited to express the benefits of recovering resources from waste, because the effect of resource provision on production processes outside the waste system is accounted for. Furthermore, the consideration of the waste's upstream burden in the exergetic LCA, as done in this study, constitutes an innovation for waste LCA and provides an indication of the waste's (maximum) resource potential, which forms a baseline for optimizing resource recovery.

2.3.5 Entropy-based assessment of P use efficiency in Austria (*Publication [17]*)

Statistical entropy analysis (SEA) was developed to evaluate the outcome of material flow analysis (MFA) with respect to a material flow systems' ability to concentrate or dilute a substance (Rechberger 1999, Rechberger and Brunner 2002). Based on the idea that entropy generation must be kept low in a resource efficient economy by transforming high-entropy wastes into low-entropy secondary raw materials, SEA has also been put forward as a measure of sustainable resource use (cf. Rechberger and Graedel 2002). In the present study *[17]*, SEA was applied to assess the efficiency of phosphorus (P) resource use in Austria. Therefore, the existing methodology was adapted to be able to account for numerous material flows in different sectors, multiple recycling loops within the system, and imports and exports at different stages. The adapted method enabled the direct use of MFA results without the need to change flow structures or quantities of the underlying material flow model. National P use efficiency was evaluated based on existing MFA studies over time (cf. Zoboli et al. 2016a) as well as with respect to a scenario of fully optimized P management (cf. Zoboli et al. 2016b). The evaluation showed that changes in P management over time had a significant effect on the resource efficiency of P use in Austria. The increase in relative statistical entropy throughout the national P life cycle decreased by a quarter between 2000 and 2010, which was mainly due to lower levels of dissipative emissions (less over-fertilization), more efficient bio-industry (food and bioenergy), and higher P removal rates in waste water treatment. These improvements outweighed the negative effect of banning the recycling of meat and bone meal (in 2001) on P use efficiency. For the optimized P management scenario, the positive effects of measures to reduce emissions, enhance recycling, and reduce consumption of P on resource efficiency (the fully optimized scenario lead to half the entropy increase compared to current P management) were reflected by the statistical entropy-based assessment. Therefore, relative statistical entropy was a suitable indicator to integrate various dimensions of resource use and served as a basis to assess and improve the resource efficiency of macro-scale material flow systems illustrated via P resource use in Austria.

The major achievement of this work was the adaption of the existing SEA framework to enable the application to complex material flow networks without prior modification of the flow structure or the flow values of the underlying MFA. Compared to the evaluation of highly aggregated (e.g. Rechberger and Graedel 2002, Yue et al. 2009) or linearized (e.g. Bai et

al. 2015) material flow schemes in the past, the adapted method can be used to evaluate the resource efficiency of real and complex substance flow systems in a straight-forward manner. Thus, relative statistical entropy (its trends and changes between different life cycle stages) can be used as a meaningful indicator on top of MFA studies to optimize resource efficiency of macro-scale material flow systems.

3 Conclusion and outlook

The transition from linear-type use and dispose economies to more circular models of resource use entails measures to reduce, reuse, recycle, energetically valorize, and safely dispose of (unavoidable) wastes. Because wastes can serve as resources in different production systems and may contain hazardous materials, identifying optimal waste solutions is a complex task, which requires a systems perspective. Material flow analysis (MFA) is typically applied to analyze the flows and stocks of materials in society. In the context of waste systems, it is used to determine waste amounts and compositions as well as the fate of materials in waste management and secondary production processes. Therefore, MFA provides the basis for assessing different waste and resource management solutions by mapping the respective flows of materials and energy. The environmental performance of a waste system can be evaluated using life cycle assessment (LCA), which assesses impacts on the environment resulting from the provision of products and services, taking into account the whole life cycle of the product. Thus, in combination, MFA and LCA represent the framework for sound and comprehensive decision support on designing environmentally optimal waste and resource systems.

3.1 Major findings of the thesis

Most of this thesis' contributions were made in the MFA domain, where significant methodological developments could be achieved (e.g. uncertainty characterization (*[1]*, *[2]*, *[3]*, *[5]*), consistency and plausibility checks (*[7]*, *[8]*), sensitivity analysis (*[6]*), dynamic modeling techniques (*[9]*, *[10]*, *[12]*) and illustrated via case studies (e.g. *[3]*, *[4]*, *[8]*, *[9]*, *[10]*, *[11]*, *[12]*) including the provision of primary data. However, research was also progressed regarding the combination of MFA with impact assessment methods. In particular, LCA was used to determine environmental impacts associated with the material and energy flows of the resource system under investigation (cf. *[13]*, *[14]*, *[15]*, *[16]*). In addition, exergy and statistical entropy methods were applied on top of MFA to test them as resource efficiency indicators for macro-scale material flow systems (*[16]*, *[17]*). Hence, in addition to the achievements in the domain of MFA, this thesis represents a major step towards the integration of MFA and LCA in a holistic framework for environmental decision support on waste and resource management.

Like any other model-based decision support tool, MFA is inherently uncertain. In order to understand the reliability of MFA outcomes, uncertainty has to be quantitatively reflected in the results based on the evaluation of input data quality and corresponding uncertainty characterization, appropriate reconciliation and propagation methods, and critical

interpretation and communication. Major findings of this thesis related to the handling of uncertainty in MFA are:

- A systematic framework for uncertainty treatment in MFA was missing. Therefore, a step-wise procedure for uncertainty analysis in MFA was put forward in *[1]* based on an extensive literature review on uncertainty handling in MFA and related fields (e.g. LCA).
- Data quality assessment and uncertainty characterization is a critical step of uncertainty analysis in MFA, because it is subjective (to some degree) and because different methods can be used to express the uncertainty about the input value being the true value. Therefore, different methods for data quality assessment and uncertainty characterization were evaluated via case studies (cf. *[3]*, *[4]*, *[5]*) and new methods were developed specifically for macro-scale MFA purposes (*[2]*, *[3]*, *[5]*).
- Data reconciliation and consistency checks between model results and independent estimates are essential to evaluate the quality and credibility of MFA results. Therefore, existing methods for data reconciliation were compared in full-scale MFA case studies (*[4]*, *[5]*, *[7]*) and flexible data reconciliation procedures were developed (*[5]*).
- In terms of mathematical framework, possibility theory was shown to be particularly well suited to express the effect of incomplete or poor-quality data on the uncertainty of MFA results compared to the traditionally used probability theory (cf. *[4]*). Therefore, methods for uncertainty treatment in MFA using fuzzy set theory were put forward in *[5]*.
- For exploratory MFA (i.e. dynamic material flow models), the identification of critical model parameters or input data, which have a large effect on the results, is of particular importance due to more complex model structure and generally higher data demand. Therefore, interaction and time-delay effects of parameter variation on the output of dynamic material flow models was investigated using global sensitivity analysis and a decision tree for appropriate sensitivity practices in dynamic MFA was developed in *[6]*.
- So far, the effect of modeler's choices on the outcome of MFAs has not been investigated, but may impede meaningful comparisons across different MFA studies. Therefore, a generally applicable approach to analyze and transparently document choices in MFA was put forward in *[7]* based on the comparison of the phosphorus budgets for Austria and Denmark.

The material dimension of resource systems dynamics is typically investigated using dynamic MFA (dMFA). Whereas material flows in a specific period (e.g. one year) are often the core subject of static MFA studies, dynamic MFA studies put the focus on the development of material stocks in society and related end-of-life flows. Major findings of this thesis related to the modeling of resource system dynamics are:

- The combination of bottom-up and top-down methods to calibrate and validate dynamic material flow models is central to increase confidence in model outcomes. Appropriate procedures were developed and implemented for a case study on Al resource use in Austria (*[8]*) and for a case study on end-of-life wood flows from Viennese buildings (*[10]*).
- Fully circular resource systems cannot be achieved within the coming decades for most materials due to consumption levels surpassing the potential supply of secondary raw materials (i.e. continuous growth of in-use material stock). This was illustrated for the hypothetical case of a closed Al cycle in Austria until 2050 from a quantitative ([9]) as well as qualitative ([11]) perspective.
- The quality of end-of-life materials does not fully conform with the demand for raw material inputs due to changes in products (i.e. different demand), contamination during use, or mixing with other materials during the end-of-life phase. This was highlighted in *[10]* with respect to legacy contaminants constraining wood recycling, in *[11]* with respect to Al alloy qualities, and in *[12]* for chemicals in paper products in Europe. In general, material quality aspects become more critical for the utilization of EOL materials with increasing recycling levels. In the case of Al, it could be shown that enhanced sorting as well as international scrap trade are suitable mitigation strategies to avoid quality constraints in secondary production.
- Establishing clean cycles and directing problematic substances into suitable sinks is a key issue of an increasingly circular economy. Therefore, the material-flow based approach for assessing chemicals contamination of product cycles developed in *[12]* is a major step towards a consistent evaluation of the environmental performance of circular product systems.

MFA is the central tool to investigate resource use patterns and identify recycling potentials as well as losses throughout the material life cycle. Based on the balancing of material flows in defined system, consistent inventories as a basis to assess the resource efficiency and environmental performance of the system under investigation are generated. Hence, in combination with LCA or other assessment methods, MFA enables the evaluation of resource systems on different scales, from plant-level to regional-level studies. Major findings of this thesis related to the evaluation of resource recovery strategies are:

- The stipulation of high recycling levels does not necessarily result in goal-oriented waste management solutions. Using EOL cooling appliances as a case study, *[13]* showed that the optimal recycling rate is a function of waste composition, the technologies available for treatment and recycling, as well as the products substituted for by secondary production.
- The environmental performance of waste systems involving waste incineration residues is often sensitive to choices concerning the handling of long-term emissions in LCA. This was highlighted by analyzing the effect of different methods

to establish the emission inventories of alternative municipal solid waste incineration fly ash treatment scenarios on their environmental impact scores in *[14]*.

- Resource recovery from closed landfills (=landfill mining) can result in a net-saving or a net-burden in terms of global warming depending on the conditions at the site. Therefore, the importance of different factors on the site, project, and system level for the climate impact of landfill mining was systematically analyzed in *[15]* to facilitate the development of climate-friendly strategies and policies for landfill mining.
- Resource recovery strategies from waste need to be based on consistent material and energy balances and should be optimized in view of different objectives. This is illustrated for resource recovery from household waste in *[16]*, where different exergy analysis methods result in different optimal resource recovery strategies. Whereas high metals recycling rates are generally beneficial, preferences with respect to energy recovery or material recycling of plastics and organic waste are dependent on the assessment method used. Therefore, the choice of assessment methods has to be reflected in the goal of the study and sensitive parameters or choices have to be critically discussed and quantitatively analyzed.
- Evaluation is an essential step on top of MFA studies to relate material flow results to societal goals such as environmental protection or resource conservation. For instance, statistical entropy is applied in [17] on top of macro-scale MFA studies to assess the resource efficiency of phosphorus use in Austria and highlight optimization potentials.

3.2 Perspectives on future research

The transition towards more circular material flow systems will further increase the interdependency between EOL flows and inputs to the production systems. In order to provide robust decision support on environmentally optimal material flow networks and recycling schemes, further research efforts are required in each of the topical areas addressed in this thesis.

In the recent years, major progress has been made concerning the handling of uncertainty in MFA by work constituting this thesis as well as by other studies (e.g. Bader and Scheidegger 2013, Cencic and Frühwirth 2015, Dubois et al. 2013, Kopec et al. 2016, Lupton and Allwood 2017, Rechberger et al. 2014). Now, the focus should shift from developing appropriate methods to implementing the theoretical state-of-the-art into easy-to-use tools. Apart from establishing uncertainty analysis as a standard element of MFA, research on suitable methods for communication and visualization of uncertain results is needed to provide significant and reliable decision support. In this context, the link between the quality of material flow data (i.e. confidence in the data) and the consistency of material flow results (i.e. degree of reconciliation) should be further explored.

The use of dynamic MFA to analyze the development of resource systems over time has increased dramatically throughout the last three decades. In order to account for increasing shares of secondary production in product systems, the simultaneous modeling of substance, goods, and product cycles in dynamic MFA to quantitatively and qualitatively account for recycling loops will evolve as a major field of future research. In particular, the consideration of impacts due to product-related exposure to „recycled“ hazardous substances and the consideration of technical material qualities in the evaluation of the resource system warrant further research (pioneering work is presented in this thesis, e.g. *[11]* and *[12]*). In general, efforts to couple material flow dynamics and life cycle impacts in a single modeling framework should be made to enable comprehensive decision support on the design of resource systems.

The environmental performance of resource recovery is typically evaluated using MFA in combination with other methods, mostly LCA. However, a tool to couple material flow model results and life cycle inventory datasets is currently missing, but would increase the consistency and transparency of MFA-based evaluations. Therefore, efforts should be made to integrate MFA and LCA models. This will assure consistency between the material flow results uncertainty and their use as inventory data of the LCA model. Furthermore, the effect of choices on product substitution on the environmental performance of resource recovery warrant further research, because they are often decisive for the outcome. Finally, the consequences of modeling long term emissions in waste management (i.e. from landfills) should be critically reflected in environmental assessments of resource recovery. In particular, related to residues associated with low emission rates over very long time periods (cf. Laner 2009). Generally, future evaluation studies should aim at creating a systemic understanding of the role of specific factors and conditions for the environmental performance of a system (similar to *[15]*) as a basis to support sustainable policy development.

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5 Appendix: Articles [1] – [17]