Doctoral Thesis

DEALING WITH UNCERTAINTY IN MATERIAL FLOW ANALYSIS

submitted in satisfaction of the requirements for the degree of Doctor of Science in Civil Engineering of the Vienna University of Technology, Faculty of Civil Engineering

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Dissertation

UMGANG MIT UNSICHERHEITEN IN DER STOFFFLUSSANALYSE

ausgeführt zum Zwecke der Erlangung des akademischen Grades eines Doktors der technischen Wissenschaft eingereicht an der Technischen Universität Wien Fakultät für Bauingenieurwesen von

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Vienna, March 2017

Acknowledgments

First of all, I would like to express my deepest gratitude to David Laner for his guidance, his encouragement, his patience, his unlimited support and great amount of effort in carrying out this research project. I learned so much about scientific work processes and reasoning in this field through all the discussion we had. It was motivating, inspiring, and a great honor to work with him. I also want to thank Helmut Rechberger for supervising my work and giving me the freedom to work on exotic mathematical methodologies deviating from the actual field of research at the department. Further, I want to say thanks to Johann Fellner for giving me the chance to be a member of the Christian Doppler Laboratory which provided me the opportunity to extend the scope and intensity of my research. I would also like to express my great appreciation to Reinout Heijungs and Didier Dubois for their evaluation.

Many thanks to all my colleagues at the institute for such a great working environment. Special thanks to Oliver Schwab, not only for having such a great time sharing the office during the last three years, but also for becoming such a good friend, and to Andrea Winterstetter, for all the serious and not so serious discussions and great laughs we had together and still do.

The work performed in this thesis was carried out within the program "Innovative Projekte" which is competitive funding program of the TU Wien with a focus on interfacultary cooperation. Furthermore, it was supported by two large-scale research projects: The IRMAR (Integrated Resource Management & Recovery) initiative funded by the Danish Research Council and the Christian Doppler Laboratory on Anthropogenic Resources funded by the Austrian Federal Ministry of Science, Research and Economy, and the National Foundation for Research, Technology and Development. The financial support of is gratefully acknowledged.

Finally, I want to thank my parents, my great friends and my boyfriend for all their encouragement and support.

Abstract

Material flow analysis (MFA) is a tool to investigate material flows and stocks in defined systems as a basis for resource management or environmental pollution control. Due to the lack of general information on data and model structure, and the diverse nature of data sources, MFA results are inherently uncertain (e.g. recycling rates, flow quantities). In this work, the treatment of uncertainty in material flow modeling is analyzed. Possible causes of uncertainty, such as uncertainty of model parameters or uncertainty of model structure, and the according treatment methods, such as uncertainty analysis, sensitivity analysis and uncertainty treatment of model structure, are presented. In order to address the typical drawbacks of uncertainty treatment in MFA in already existing approaches, three studies with three methods, differing in problem set-ups and objectives, are proposed in this work.

As various MFA studies rely on data about flows and stocks from different sources with varying quality, in the first study, an uncertainty analysis method, which expresses the belief that the available data are representative for the value of interest via fuzzy sets, is presented, specifying the possible range of values of the data. A possibilistic framework for data reconciliation in MFA was developed and applied to a case study on wood flows in Austria. The framework consists of a data characterization and a reconciliation step. Membership functions are defined based on the collected data and data quality assessment. Possible ranges and consistency levels (quantifying the agreement between input data and balance constraints) are determined. The framework allows for identifying problematic data and model weaknesses, and can be used to illustrate the trade-off between confidence in the data and the consistency levels of resulting material flows.

While reconciliation is useful in static MFA systems, the focus in dynamic MFA system is rather on robustness of the material flow models, by defining variation ranges for parameters rather than to capture the true range of variation. Therefore, the use of sensitivity analysis in dynamic MFA studies has been on the increase. Variance based global sensitivity analysis decomposes the variance of the model output into fractions caused by the uncertainty or variability of input parameters. The second study investigates interaction and time-delay effects of uncertain parameters on the output of an archetypal input-driven dynamic material flow model using variance based global sensitivity analysis. The results show that determining the main (first order) effects of parameter variations is often sufficient in dynamic MFA because substantial effects due to the simultaneous variation of several parameters (higher order effects) do not appear for classical set ups of dynamic material flow models. For models with time-varying parameters, time-delay effects of parameter variation on model outputs need to be considered,

potentially boosting the computational cost of global sensitivity analysis. Finally, the implications of exploring the sensitivities of model outputs with respect to parameter variations in the archetypal model are used to derive model- and goal-specific recommendations on choosing appropriate sensitivity analysis methods in dynamic MFA.

When it comes to dynamic studies of uncertain model structure, sensitivity analysis may not be sufficient. Principal examples are analyses of waste streams of building stock, which are uncertain with respect to data and model structure. Wood constructions in Viennese buildings serve as a case for the third study to compare different modeling approaches for determining end-of-life (EOL) wood and corresponding contaminant flows (lead, chlorine and PAH). A delayed input and a leaching stock modeling approach are used to determine wood stocks and flows from 1950 until 2100. Cross-checking with independent estimates and sensitivity analyses are used to evaluate the results' plausibility. Under the given data situation in the case study, the delay approach is a better choice for historical observations of EOL wood, and for analyses on a substance level. It has some major drawbacks for future predictions on the goods level, though, as the durability of the high amount of historical buildings with considerably higher wood content is not reflected in the model. The wood content parameter differs strongly for the building periods, and has therefore the highest influence on the results.

Author's contribution

The results of three years of research are put together in this thesis. It builds upon three journal articles (which can be found in the Appendix of this work):

Article I:
A fuzzy set-based approach to data reconciliation in material flow modeling
Nađa Džubur, Owat Sunanta, and David Laner
Applied Mathematical Modelling, 43 (2016)

Article II:
Evaluating the Use of Global Sensitivity Analysis in Dynamic MFA
Nađa Džubur, Hanno Buchner, and David Laner
Journal of Industrial Ecology, 20 (2016)

Article III:
Evaluation of modeling approaches to determine end-of-life flows associated with buildings: a Viennese show case on wood and contaminants
Nađa Džubur and David Laner
Journal of Industrial Ecology, under revision.

I primarily contributed to the three articles, including the problem framing, performance of analysis, interpretation of results and drafting. David Laner has contributed to the research design by helping me to find the right problems to develop my solution methods. He was also involved in all steps of the three articles with important inputs, such as productive ideas, detailed comments and critics. Owat Sunantna contributed with detailed comments on the theoretical part of Article I. The problem of Article II arose out of work done by Hanno Buchner. Apart from helping me to frame the problem, he was also involved in the interpretation of the results and helped me to compare them by applying the EASI algorithm on the problem.

Contents

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List of abbreviations

C&D waste Construction and demolition waste

EOL End-of-life

FAST Fourier amplitude sensitivity test

EASI Effective algorithm for computing global sensitivity indices

LCA Life cycle assessment

MFA Material flow analysis

MMFA Mathematical material flow analysis

SFA Substance flow analysis

OAT One-at-a-time

PAH Polycyclic aromatic hydrocarbons

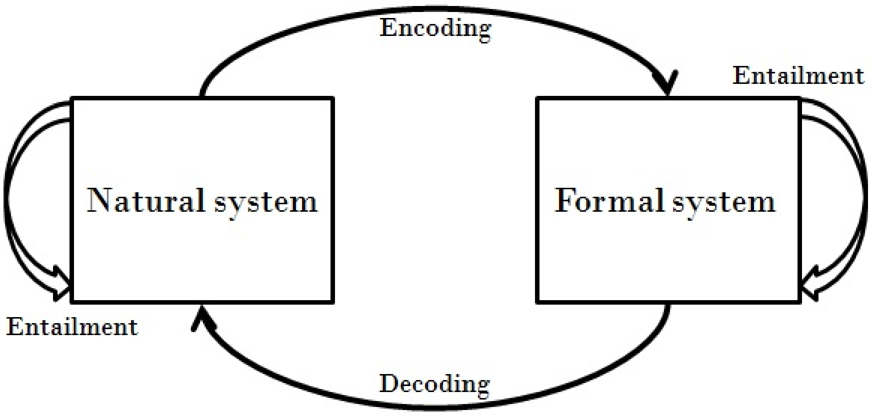
1 Introduction

1.1 Scientific modeling

1.1.1 The meaning of models

Taken from the work of biologist Robert Rosen (1991), the world, the subject of our investigations, can be seen as a natural system which is governed by rules that we want to uncover. Therefore, a set of structures is hypothesized and transformed into a formal system or model, which is a theoretical construct building the abstract representation of a natural system (see Figure 1.1). Models form the basis of scientific theory. Rosen states that while the world obeys its rules which contain internal entailments, and while the model follows some mathematical or formal rules, containing also internal entailments, there is no entailment of the world to the model. One of the reasons for this paradox is the fact that the proportion of the world captured by the model is an arbitrary enclosure of an otherwise open system. However, experience has shown that even if the natural

Figure 1.1: Modeling after Rosen (1991)



system is indeed a well-defined and closed one, different modelers can generate different nonequivalent descriptions of it, so that the structures are not reconcilable with one another. The term equifinality, defined by Beven (1993, 2000), describes this phenomenon of different models where same observations lead to the same end. Others also refer to this as indeterminancy. The development of laws to deal with the limited capacity of the human mind to create a useful mapping of the world as a natural system into a formal system of a model is a labored process of simplification, separation and identification, making modeling a design problem. There is not a unique, true model of a natural system. Different models are adequate to address different sets of scientific questions. Which aspects of a natural system should be described in more detail and which in a more aggregated way (cf. Saltelli et al. 2000; Saltelli et al. 2004; Saltelli et al. 2008; Reichert 2014) depends on the purpose of the model application, on the available data, and on the effort which can be put in the model development.

Models can either be used to improve our understanding of the structure and function of a natural system or to predict future behavior in support of management. Models to answer scientific questions can be constructed by following guidelines (based Spriet 1985, adapted by Reichert 2014): (1) Causality, meaning the model structure should represent the relevant cause-effect relationships at the required level of resolution, (2) universality, meaning that the model should be as transferable as possible from one system to another, (3) predictive capability, meaning that the model should remain valid for extrapolation of external influence factors for a predictive use, (4) identifiability, meaning that the values of unknown parameters should be identifiable to an adequate accuracy, and for predictive capability, prior knowledge about non-identifiable parameters should be available, (5) simplicity, meaning that the model should be as simple as possible with the requirements formulated above, avoiding unnecessarily complicated descriptions. Future predictions in modeling can either be made by extrapolation of results of a model representing the major casual relationships, or by a phenomenological model (Reichert 2014).

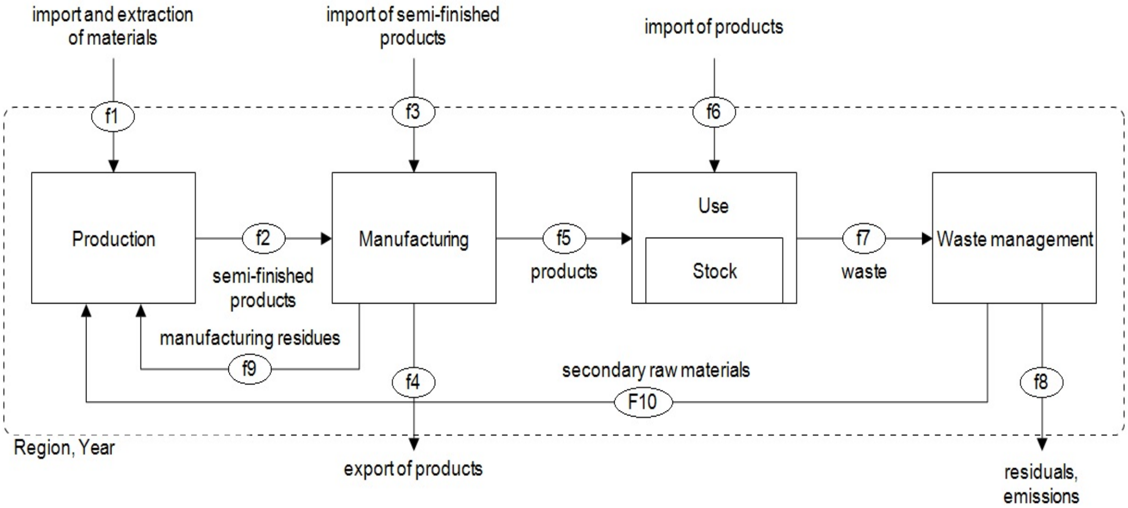
1.1.2 Material flow analysis

Method

An example of modeling a natural system is material flow analysis. Anthropogenic systems are defined as the habitat of mankind together with all technical and biological processes built and driven by man, and spaces where his activities take place. The complementary part to the anthroposphere is designated as the environment (which is driven by nature). The anthroposphere interacts with the environment via extraction of resources and wastes and emissions of off-products. Based on Leontief's input-output table methodology to quantify mutual interrelationship among various sectors of a complex economic system (Leontief 1977), MFA has been developed in the 80s and 90s to describe the metabolism of the anthroposphere. MFA is an analytical method for the assessment, interpretation and description of mass balance systems (Baccini and Brunner, 1991). Main publications on MFA include Baccini and Bader (1996), Brunner and Rechberger (2004), Baccini and Brunner (2012), and van der Voet et al. (2002). The method assesses the state and changes of flows and stocks of materials within a system defined in space and time, connecting the sources, the pathways and intermediate sinks of a material. If a specific substance is the focus, MFA is sometimes also referred to as substance flow analysis (SFA). As the results can easily be compared by checking the inputs, outputs and stocks of processes within the system through a simple mass balance, MFA is an attractive decision support tool in resource management, waste management, environmental management, and policy assessment (Brunner and Rechberger 2004, 2014). It has been widely applied to investigate resource and recycling systems, providing useful information regarding the patterns of resource use and loss of materials into the environment (e.g. Gradel et al. 2004; Modaresi and Müller, 2012; Ott and Rechberger, 2012; Zeltner et al. 1999; see also Laner et al. 2014).

General definitions are used to define MFA systems. Material is used as a term for substances and goods. Substances are elements or compounds composed of uniform units. Goods stand for entities of matter which have an economic value by markets. They are made up of one or several substances. A process is a transport, transformation or storage of materials. Stocks are parts of processes that store the mass of materials within the analyzed system. They can stay constant, increase (accumulation of material) or decrease (depletion of materials). Processes are linked by flows of materials, which transport mass per time unit. Flows across system boundaries are called imports or exports. Flows that enter a process are denoted as inputs, while flows that exit a process are outputs. Transfer coefficients describe the partitioning of a good or a substance in a process. The system comprises a set of material flows, stocks and processes within a defined boundary, set in space and time (Brunner and Rechberger 2004, 2014). A simple, generic MFA model is given in Figure 1.2. The system boundaries are defined for a specific region for a year. The model consists of the processes Production, Manufacturing, the Use-phase with a stock storing materials in use, and the Waste management within the region. The flow of semi-finished products is transferred from the Production to the Manufacturing process and the flow of products from the Manufacturing into the Use-phase process. In the Use-phase, materials remain in stock until their lifetime is over, and finally end up as waste flows in the Waste management. Some materials may

Figure 1.2: Generic MFA model



be recycled, thus, there is a flow of secondary resources from the Waste management entering the Production process again. Furthermore, there is a flow of recycled residues from the Manufacturing going back into the Production process. Input flows across the boundaries are the import from materials from other regions, or extractions from the environment within the primary production, which in this example are the import of semi-finished products in the Manufacturing, and the import of products in the Use-phase. Output flows across the boundaries are exports of manufactured products into other regions or emissions and residuals going into the environment. Flows, stocks and transfer coefficients are underlined with input data as far as it is available. Unknown and overdetermined flow quantities are calculated through the mass balances defined by the processes.

Classification of MFA models

Consistent and complete information is provided by MFA within the defined system boundaries in space and time. The design of the model depends on the purpose and general framework. MFA studies can either be static, describing a snapshot of a system in time, or dynamic, describing the behavior of a system over a time period (Chen and Graedel, 2012). MFA can be done on a national or regional scale (material flow accounting, see Fischer-Kowalski et al. 2011), where material exchanges between an economy and the natural environment are analyzed. Furthermore, MFA can be done along an industrial supply chain to quantify and optimize the production processes of

companies (Material flow cost accounting, see Wagner et al. 2010).
Material stocks of processes can be identified by two different methods. The top-down approach is a method which derives the stock from the net flow, i.e. the difference between inflows and outflows. The other method is the bottom-up approach. This method directly estimates the stock by summing up materials which are pertained within the present system boundary at a certain time (Gerst et al. 2008). While static MFA studies are rather based on bottom-up observations of the stock (offering a more precise foundation for the analysis), dynamic MFA studies are usually based on a top-down approach due to the high expenses of bottom-up studies.

Limitations

While MFA is insightful in principle, the reliability of the results has been questioned due to data limitations and inherent uncertainties in the analysis (Danius and Burström, 2001). As MFA concerns gathering, harmonizing and analyzing data about physical stocks and flows from various different sources with varying quality, limitations of data are unavoidable in material flow studies (cf. Chen and Graedel, 2012). Despite this, uncertainty is often disregarded in MFA, or at best limited to a qualitative discussion of validity of the results (e.g. Lifset et al. 2012). However, the consideration of uncertainty is receiving increasing attention in recent years in applied studies (Laner et al. 2014).

1.2 Description of uncertainty

As already indicated in the previous chapter, a model can never perfectly represent a natural system. Because of that, model predictions are always uncertain (Reichert 2014). Modelers and philosophers of science have debated the issue of model indeterminacy at length (Oreskes et al. 1994). Most of the modelers today agree that a model cannot be validated in the sense of being proven true, but rather, they would say, it has been extensively corroborated, meaning the model has survived a series of testing, either formal, of internal consistency, or relative to the model's capacity to explain the world in a convincing way (Saltelli et al. 2008). Sources of uncertainty can either be of aleatory or epistemic nature. Aleatory uncertainty is often also referred to as variability. It is caused by randomness and cannot be reduced by knowledge. Epistemic uncertainty is caused by a lack of knowledge and can be minimized through further examination (cf. Ferson and Ginzburg 1996).
Models do often occur in highly polarized contexts, thus, uncertainty may be used instrumentally (Saltelli 2008). Literature on how to deal with uncertainty in quantitative

risk and policy analysis is given by Morgan and Henrion (1990) and for science in policy by Funtowicz and Ravetz (1990).

1.2.1 Causes of uncertainty

The causes of uncertainty can be non-deterministic behavior of a system (a), uncertainty of model parameter values (b), uncertainty of model structure (c), uncertainty due to external influence factors (d), and finally, uncertainty due to numerical solutions of model equations (e) (Beck 1991, modfied by Reichert 2014).

(a) Non-deterministic behavior of a system
Non-deterministic behavior of a system is usually due to chaotic behavior rather than due to true randomness at a macroscopic level. Chaotic behavior denotes deterministic systems which are very sensitive to initial conditions. As the initial state of a system can never be reproduced in full, this leads to observed non-deterministic behavior. Besides this, there are also other causes of non-deterministic behavior which can be well described by random model elements, such as aggregation errors. As chaotic behavior, this is due to epistemic uncertainty as there is a lack of spatial resolution. Another reason of non-deterministic behavior can be influence factors, which cannot be measured and therefore, cannot be considered in a model.

(b) Uncertainty of model parameter values
The usage of model parameters can specify the essential structure of dependence in the model. Still, there remain unknown model variables that must be adapted empirically. Parameter estimation should not only provide the best estimates of model parameters, but also of their uncertainty, which can be propagated in the results.

(c) Uncertainty of model structure
Structural model errors may consist of an inadequate selection of model variables and processes, an inadequate selection of process formulations, or an inadequate formulation of spatial and temporal resolution of a model. Such errors are not easily quantifiable.

(d) Uncertainty due to external influence factors
External influence factors describe the influence of the environment on the considered system.

(e) Uncertainty due to numerical solutions of model equations
Usually, model equations must be solved numerically. The accuracy of these numerical solutions is usually much higher than uncertainty due to other sources, and can often be neglected. An exception is the usage of Monte Carlo simulation techniques to calculate probability distributions, the use of which can lead to significant errors in the results if the number of runs is too low. Other potential causes of uncertainty can be the use of poor numerical techniques (see Clark and Kavetski 2010).

1.2.2 Uncertainty in MFA

MFA relies on data about flows and stocks from different sources with varying quality. Because of the lack of direct observations of quantities that are of interest, data are often taken from alternative sources of even more varying qualities. Thus, MFA is naturally confronted with model parameter uncertainty, to which degree the available data captures the true values of the variables (flows and changes in stock) of the system under investigation. The use of quantitative methods to handle uncertainties of model parameter values in MFA has received increasing attention in recent years in applied studies (e.g. Bader et al. 2011; Do-Thu et al. 2011; Gottschalk et al. 2010; Hedbrant and Sörme 2001; Huang et al. 2007; Ott and Rechberger 2012; Bonnin et al. 2013; Klinglmair et al. 2016; Laner et al. 2016) as well as in studies explicitly addressing issues of uncertainty analysis in MFA (e.g. Gottschalk et al. 2010; Hedbrant and Sörme 2001 (cf. Laner et al. 2014); Laner et al. 2016; Schwab et al. 2016).
Aleatory uncertainty can be appropriately handled with concepts used for describing observed frequencies of random events (frequentist approach) while epistemic uncertainty requires concepts for dealing with the degree of belief in data or reasonable assumptions reflecting available data (subjective approach, cf. Reichert 2014). These two types of uncertainty are typically confused in MFA, making it difficult to distinguish what is known from what is assumed. In addition to that, the application of mathematical procedures for propagating uncertainties is sometimes inconsistent with the data characterization concept of the MFA study. The convenient assumption that uncertain quantities are independent and normally distributed (e.g. in STAN, see Cencic and Rechberger 2008) may lead to drawbacks, as normal distributions cannot limit the range of possible values to only positive quantities, which are typical for MFA (Laner et al. 2014; Laner and Cencic 2013).

Other sources that typically arise are of structural nature, related to the mathematical model, or uncertainty of external factors, due to assumed scenarios (errors due to inappropriate use of numerical solutions of Monte Carlo techniques are unusual). Both types of uncertainty are typically ignored in MFA.

1.3 Treatment of uncertainty

1.3.1 General methods

As already mentioned, models are simplified descriptions of reality and therefore, there is no unique description of a natural system by a mathematical model. Which model provides the adequate description depends on the purpose of modeling. In order to address different questions, there is a need for different levels of resolution. Nevertheless, in order to enable deriving estimates of uncertainties, any model must be based on a solid statistical foundation (Reichert 2014). If a model is constructed, and various uncertainties in the inputs are identified, it is important to discover the propagation of these uncertainties throughout the model (for both, quantitative outputs depending on the inputs, and decision variables depending on quantities). The modelers should be able to obtain useful insights about the relative importance of the various assumptions, decisions, uncertainties, and disagreements in the inputs to the conclusions. These insights can be helpful to decide whether it is likely to be worthwhile to gather more information in order to make more careful uncertainty assessments, or to redefine the model, and which of these decisions could cause the highest reduction of uncertainty (Morgan and Henrion, 1990).
Different methods for the treatment of different types of uncertainty are provided: Uncertainty analysis is performed in order to quantify the range of possible output outcomes (e.g. indicators), given a set of uncertain inputs. A related practice is sensitivity analysis, which is the study of how uncertainty in the output can be apportioned to different sources of uncertainty in the model input. It describes how sensitive the output is to variation of individual, or groups of, input parameters (Saltelli et al. 2008). While these methods are based on statistics, uncertainty about the model structure can only be minimized by qualitative comparisons. An exception is given if uncertainty occurs only in specific functions of a model. This can be treated with some kind of sensitivity analysis by identifying a metamodel and treating functions as sensitive inputs and varying them in scenarios (Morgan and Henrion, 1990). Furthermore, validation with independent cross-check data can be useful to identify uncertainties in models.

1.3.2 Methods used in MFA literature

Methods to deal with uncertainty in MFA range from qualitative discussions to sophisticated statistical approaches. The focus of this work is put on methods which include a mathematical treatment of uncertainty in MFA (based on calculations involving different types of uncertainty and not only on mapping the flows). The majority of methods can be classified into four groups: data classification methods, uncertainty analysis approaches, sensitivity analysis approaches, and comparisons of model structures.

Data classification
There are three kinds of data classification approaches. An approach to harmonize societal data where uncertainty intervals are determined is given by Hedbrant and Sörme (2001). Depending on the data structure and the specificity, they derived uncertainty levels for MFA data. Asymmetric intervals are calculated by assigning uncertainty factors to each uncertainty level. Lassen and Hansen (2000) use probability distributions to represent uncertain values and indicate the uncertainty with symmetric intervals. Another method to classify data used in LCA is the pedigree matrix by Weidma and Wesnaes (1996). This matrix consists of five independent data quality indicators which are used to communicate data limitations and could be used in MFA as well (see also Laner et al. 2014). A quantitative method based on quality indicators and information theory ("information defects") used in MFA is presented by Schwab et al. (2016).

Uncertainty analysis
Several probability approaches to deal with uncertainty in MFA are already in use. Cencic and Rechberger (2008) propose the widely used MFA software STAN, which is a ready-to-use tool for doing MFA while taking into account uncertainty. Uncertain data is specified as the mean and standard deviation of a normal distribution. Analytical calculation of error propagation and data reconciliation for overdetermined systems are performed with STAN. As already mentioned above, the usage of normally distributed functions for uncertain data of non-frequentist behavior has some major limitations. Taking into consideration the possibility that material flow data may not be normally distributed, recent work was done by Cencic and Frühwirth (2014) to perform data reconciliation of data with more general probability distributions in linear material flow systems. The study is based on Bayesian statistics. A further approach based on Bayesian statistics is provided by Gottschalk et al. (2010). Prior probability distributions are defined using the knowledge about model parameters, and, based on the observed data, posteriors are derived using Monte Carlo sampling. From these posteriors, the uncer-

tainty of a flow is estimated. The mathematical material flow analysis approach (MMFA) by Bader et al. (2011) has similarities with a Bayesian approach. Uncertain model parameters are specified using different kinds of probability density functions. In contrast to a Bayesian setting, in this approach, the mathematical functions are fitted to the available data. Therefore, it is also an approach on fitting the model structure. Monte Carlo sampling is used in this approach, too, to estimate the output and calibrate the model, as well as sensitivity analysis to identify critical parameters (Laner et al. 2014). As aleatory and epistemic uncertainty should be distinguished and treated differently (Refsgaard et al. 2007; Ferson and Ginzburg, 1996), which cannot be done with probability functions, alternative representations of uncertain quantities of epistemic nature in environmental assessment models using interval concepts (Chevalier and Teno, 1996) and possibility (fuzzy set) theory (Clavreul et al. 2013, Guyonnet 2012, Holtmann et al. 2005, Tan et al. 2007) were put forward. So far, in an MFA context, fuzzy reconciliation approaches have been compared to the standard least squares approach to quantify material flows of resource and recycling systems (in Dubois et al. 2014; Laner et al. 2015).

Sensitivity analysis
In contrast to uncertainty analysis, approaches focusing on sensitivity analysis analyze the effects of parameter uncertainty or variations on the model results relatively, without trying to capture the true range of variation. As this facilitates the definition of uncertainty of parameters and the range within they may vary, and puts the focus on evaluating the robustness of the material flow model, this type of approach has been frequently applied to dynamic material flow models (Laner et al. 2014). The common way to treat dynamic MFA in previous literature is local, using one-at-a-time (OAT) analysis, where one input variable is changed while the others remain fixed in order to see what effect this produces on the output (Murphy et al. 2004). The outputs are analyzed through Monte Carlo Simulation. MFA studies using local sensitivity analysis and considering uncertain data are done by Glöser et al. (2013), Gottschalk et al. (2010), Tsai and Krogmann (2013), Spatari et al. (2005), Zeltner et al. (1999), Ruhrberg (2006). Such a treatment is very time-consuming if the system consists of many inputs, which need to be observed. Further, local OAT analysis cannot account for the combined effects of parameter changes so that interaction effects attributed to the simultaneous variation of parameters are ignored. Whereas local sensitivity analysis methods focus on testing different perturbations of (constant or uncertain) input parameters and analyze the specific consequences in the output, global sensitivity analysis focuses on the uncertainty in the output and how it can be apportioned to different sources of uncertainty in

the inputs (Saltelli et al. 2008). Bader et al. (2011) used both, global and local sensitivity analysis to investigate an MFA model by focusing on specific stock saturation-based scenarios. McMillan et al. (2010) present a more specific application of global sensitivity analysis to model stocks and their relationship with economic output. They used a Fourier amplitude sensitivity test (FAST) to identify not only the main effects, but also interaction effects of parameter variations. Buchner et al. (2015) explored the variations in the output by applying Sobol indices for main effects using the effective algorithm for computing global sensitivity indices (EASI, by Plischke 2010). The EASI algorithm is, like the FAST algorithm, based on Fourier transformations.

Comparison of model structures
As already mentioned, comparisons of model structures are rare in MFA. A comparison of model structures of the Austrian and Danish phosphorus balance systems is given by Klinglmair et al. (2016). The differences in system boundaries and definition of flows and processes are highlighted and data reconciliation is used to define a measure of model quality. Pauliuk et al. (2013) compared three different approaches of material balance equation systems to quantify the global steel cycle. The comparisons in both studies are done qualitatively. A comparison of a leaching stock approach and delay approach for dynamic SFA is given in Kleijn et al. (2000). The analytical calculation of the steady state between the mentioned two modeling approaches is given by van der Voet et al. (2002). This study presents analytical conditions under which the calculations of the leaching approach will produce acceptable solutions for dynamic models which should typically be solved using the delay approach.

1.4 Objectives and problem statement

Ignoring uncertainty aspects in material flow studies has raised doubts about the reliability of MFA results in the past. Precise considerations of uncertainty should therefore receive more attention by systematically applying appropriate approaches. The consideration of uncertainty in MFA should enable the use of all available information about the system, reflecting the purpose of the study and the data quality (Laner et al. 2014). The major problems this work should process are:

- How can uncertain MFA models be improved through a proper consideration of uncertainty in order to represent the goal of the study best?
- Which methods of uncertainty treatment are the most effective in which case at

least expenses? How can critical parameters be identified at least expenses?

- What are the limitations of existing methods for the treatment of uncertainty in MFA?
- Which method can be recommended to perform uncertainty analysis?
- Which method can be recommended to perform sensitivity analysis?
- Which method can be recommended to analyze the uncertainty of model structure?

In order to address these problems, three cases of MFA studies are presented, differing in systematic properties and modeling objectives, to show the appropriate treatment of uncertainty in each case. The overall aim of this work is to provide decision support on how to set up an MFA model with regard to uncertainty consideration.

2 Methodology

2.1 Motivation of studies

In the following section, novel possibilities are presented to deal with uncertainty in MFA. As flows and processes of MFA studies on a plant level are typically robust compared to regional studies due to data availability and structural knowledge, the focus is put on studies on a regional level. Three studies are presented, involving all categories of MFA uncertainty treatment that were mentioned in the previous chapter.

The first study shows a static, overdetermined MFA system with various data sources, conversion factors and transfer coefficients. A critical sector of the Austrian wood balance is chosen, as wood has limited data availability and imprecise information due to the vagueness of the efficiency of wood processing in various industries, the variety of wood trade units and vague data on the management of the valuable waste wood flows. Because of these various origins of inconsistencies and epistemic uncertainties, this study is an ideal resource to present a novel approach on data reconciliation using fuzzy set theory to characterize the data, balance the model, and to perform further gross error detection in order to evaluate the plausibility of model results. An adaptation of the approach of Hedbrant and Sörme (2001) is used for the data assessment step in advance. The framework allows problematic data and model weaknesses to be identified.

In contrast to the first study, the second study is dynamic, making data reconciliation difficult and confusing. This is because the flows from every time period depend on the flows from the previous period, so that the number of flows which would need to be reconciled at once is large and the source flow of changes in reconciliation is not traceable any more. The identification of critical parameters is important to get an understanding of dynamic studies, especially if recycling loops are considered, like in the case of various metal studies. The critical part of dynamic studies, especially metal studies, is uncertainty on how to aggregate and classify the products in the in use stock with regard to their lifetimes, as there are plenty of products and not all of them can be modeled individually. Therefore, global sensitivity analysis is evaluated on a reduced archetypal model consisting of lifetimes and in use stocks based on the dynamic national aluminum model. The implications of exploring the sensitivities of model outputs with respect to main and combined parameter variations with considering also delay effects are used to derive model- and goal-specific recommendations on choosing appropriate sensitivity analysis methods in dynamic MFA.

In some cases of dynamic MFA studies the observation of critical parameters is not sufficient as not only the parameters but also the model structure is disputable. Therefore, the focus of the third study is on the modeling structure of the dynamic building stock of Vienna as lifetimes of buildings vary strongly and their date of destruction or renovation may rather be driven by economic factors than technical lifetimes. A delayed input and a leaching stock modeling approach are used to determine wood stocks and flows, and contaminants from the historical building stock. The longevity of buildings, and thus, the long residence time of their potential resources in stock, may lead to an aggregation of contaminants in the stock, which may pose quality constraints for future recycling activities. As the substance level adds even more uncertainty to the already highly uncertain models, cross-checking with independent estimates and sensitivity analyses are used to evaluate the results' plausibility. The knowledge is used to derive general recommendations for waste flows of buildings on the goods together with the substance level.

2.2 A fuzzy-set based approach for data reconciliation in static material flow modeling

This chapter is based on Article I: "A fuzzy set-based approach to data reconciliation in material flow modeling" by Džubur et al. (2016). Detailed information can be found in the article in the appendix.
The basic principle of MFA is the law of mass conservation. Therefore, the sum of inputs needs to be equal to both the sum of outputs and potential changes in stock for every process in the model (cf. Equation 2.1). Flows and changes in stock for each process are the unknown variables within the system which need to be balanced by linear equations of the form:

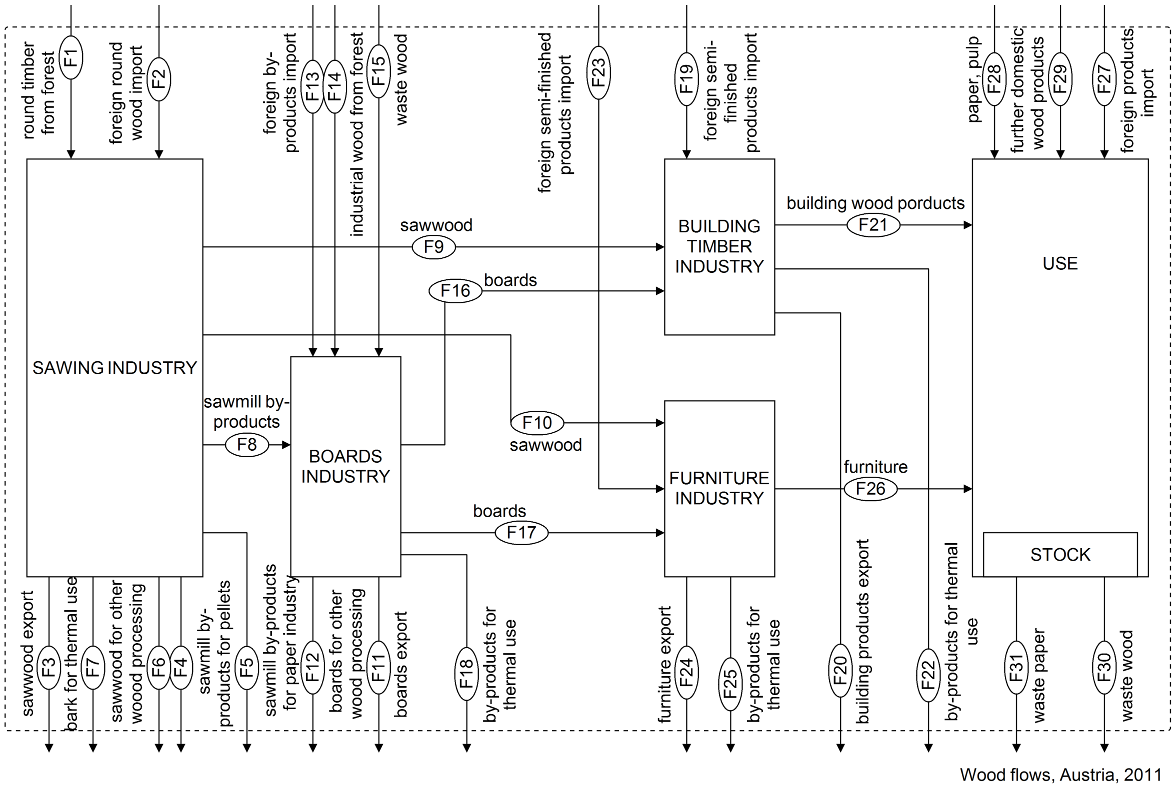
$$\sum_{i=1}^{n} f_{in_i} = \sum_{j=1}^{m} f_{out_j} + \Delta s \tag{2.1}$$

where Δs is the stock change (Δs <0 if the outflow exceeds the inflow) (see Dubois et al. 2014). In order to balance the material flows and changes in stock in the system, data need to be collected, typically originating from various sources with different data generation methods, quality standards and reporting schemes (Laner et al. 2014). If the number of unknown variables (= no input data available) is smaller than the number of balance equations, inconsistencies between input data may arise given the mass balance constraints of the model. In such cases of overdetermined systems (which are typically of static nature), data reconciliation can be used to balance the model and to further gross error detection in order to evaluate the plausibility of model results (Laner et al. 2015). Traditionally, data reconciliation in MFA is performed by minimizing the squares of measurement adjustments (using the least squares method, see also Bader and Baccini (1996), implemented in the widely used software STAN (Cencic and Rechberger, 2008). As already mentioned in chapter 1.3.2, Cencic and Frühwirth (2014) published a study based on Baysian statistics to perform data reconciliation, as the usage of normal distribution (like in STAN) may not always be the best choice of distribution. However, in situations of vague information, the choice of specific probability density functions cannot be justified in many cases, and fuzzy set theory has been put forward (cf. chapter 1.3.2). Possibility theory, originally introduced by Zadeh in 1965 to provide a graded semantics to natural language statements, is a way of reasoning in the presence of uncertainty, by expressing non-precise information with the use of membership functions (instead of probability density functions) by means of uncertainty characterization and quantification (Dubois and Prade, 1988). So far, in an MFA context, fuzzy reconciliation approaches have been compared to the standard least squares approach to quantify material flows of resource and recycling systems (Dubois et al. 2014, Laner et al. 2015). These existing applications build on linear membership functions (either triangular or trapezoidal) to characterize the given flow variables within the reconciliation approach. However, because given flows in MFA are often calculated by combining several data (e.g. amount of a commodity multiplied with the concentration of the material under investigation), the use of linear membership functions to describe flow variables is a limitation for the translation of available information to the fuzzified flow variables (cf. Laner et al. 2015). Therefore, the goal of this study was to develop a generalized approach to data reconciliation in a possibilistic framework based on fuzzy input data and fuzzy balance constraints. The approach is able to rigorously deal with multiple input data for a single flow as well as overdetermined equation systems of the material flow model and allows for arbitrary membership functions. The benefit of the generalized fuzzy reconciliation approach for improving the underlying material flow data and for evaluating the quality of the material balances is illustrated via a case study on wood flows in Austria.

2.2.1 Case Study

The focus of the case study is on a subsystem of the Austrian wood system for one year. It consists of five processes, namely the Sawing industry, the Boards industry, the Building timber industry, the Furniture industry, as well as the Use-phase of wood products containing the in use stock (see Figure 2.1). Other related processes, which are linked to

Figure 2.1: Wood Flow model for Austria in 2011 [Source: I]



the investigated system by flows, are defined to be outside of the system boundary and the import and export flows connecting them are denoted as external flows. The flows within the system boundary are denoted as internal flows. Various data sources were used and the quality of the data varies significantly. Some numbers are based on rough estimates, e.g. wood products, in which the wood content is unclear. Other sources, such as the imports of the sawing industry which are given in National statistics, are precise and reliable. As the system needs to have the same unit for balancing in order to perform data reconciliation (to obey the mass conservation law), some unit conversions are required. Some flows are overdetermined as 2-3 sources are available, and the only variable remaining unknown is the stock change Δs in the use-phase.

2.2.2 Data quality assessment

Four levels are assumed for the quality assessment, taking into consideration reliability of the source as well as representativeness. By means of those levels, the uncertainty factor u_f is computed for each collected data point according to the method of Hedbrant and Sörme (2001). The uncertainty factors have a direct influence on the quantitative uncertainty of a date as the value d

$$\frac{(u_f - 1)}{2} = d, \tag{2.2}$$

which defines the range of the fuzzy sets is calculated out of the uncertainty factor.

2.2.3 Fuzzy set theory

A fuzzy set is a generalized version of a classical set, where each value either belongs to the set or not. Every fuzzy set A^* is well-defined by its membership function

$$\xi_{A^*} : M \rightarrow [0,1], \tag{2.3}$$

mapping every value in M onto its "degree of belonging" to A^*. The interval

$$supp(x^*) := \{x \in \mathbb{R} : \xi(x) > 0\} \tag{2.4}$$

is called the support and

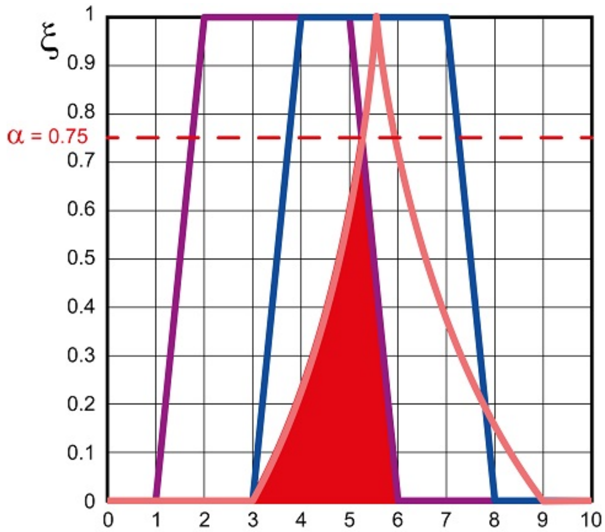
$$cr(x^*) := \{x \in \mathbb{R} : \xi(x) = 1\} \tag{2.5}$$

the core of the membership function. The support covers all possible values for a fuzzy number, whereas the core represents those values with complete membership. The maximal value of the intersection of various membership functions $\xi_1, ..\xi_n : \mathbb{R} \rightarrow [0,1]$,

$$\alpha = max_x\{min_x\{\xi_1(x), .., \xi_n(x)\}\} \in [0,1], \tag{2.6}$$

is known as the degree of consistency. An illustrative example on the maximum level of the intersection ξ^* of three membership functions ξ_1, ξ_2 and ξ_3 is given in Figure

Figure 2.2: The degree of consistency α [Source: I]



2.2. Fuzzification generalizes a crisp (discrete) number and transforms it into a fuzzy (continuous) form by determining a range of possible variation for the support and a range of highly possible variation for the core. De-fuzzification transforms fuzzy numbers into crisp numbers. Fuzzification and de-fuzzification are used in interval-based reconciliation.

2.2.4 The reconciliation model

Uncertainty characterization

The usage of an explicit function to derive uncertainty ranges guarantees a consistent characterization because it defines a transparent relationship between uncertainty scores and quantitative uncertainty estimates. According to the range d for each level, the previously categorized data is fuzzified for each flow in the mass balance system by defining membership functions of either trapezoidal or triangular shape. The input data are categorized as either quantities, conversion factors, or commodity distributions to allocate percentual shares of aggregated quantities to the flows.

Uniquely defined quantities are defined as trapezoidal functions, whereby the interval $[x \pm d \cdot x]$ is the core and the interval $[x \pm 2d \cdot x]$ is the support. Conversion factors and commodity distributions have triangular membership functions where the support is defined in the same way and the core is just the given data point x. In order to convert a flow to the unit of the mass balance system, or to assign a flow with the share of a common, aggregated quantity representing several flows respectively, the quantity is

transformed by multiplying its membership function with the function of the conversion factor (and the one of the commodity distribution respectively). The resulting function is usually neither trapezoidal nor triangular, but rather of a curved shape.
Overdetermined flows are treated by data fusion. This means, if one of the data sources (or its fuzzified version) considers a value as possible, it remains possible in data fusion (disjunctive approach, cf. Destercke 2014). Either the data are homogenous, meaning of the same unit or without the usage of a commodity distribution, then, they are merged together into a trapezoidal interval. Otherwise, the data points are harmonized before, meaning that they are defined as distinct fuzzy intervals, transformed through multiplications with either fuzzy intervals of conversion factors or commodity distributions, and then merged together by summing up over the membership functions.

Balancing of the model and the data

In the end, every flow is represented by a single membership function based on the available input data. The membership functions of the input data have to comply with the mass balance constraints given in the model. The membership functions resulting from the balance constraints are obtained for each flow by assuming that the target flow is not determined and inserting all other input membership functions for the flows belonging to the same process into the balance constraint in order to calculate it. Thus, the reconciled fuzzy intervals are calculated via intersection of the membership function of the input data with the membership function(s) from the balance constraints and the degree of consistency (α-level) is determined. Two ways of calculation can be distinguished, the first to be treated are internal flows, and external flows in a next step. The idea of the procedure is given in Figure 2.3 and Figure 2.4. The first example (Figure 2.3) shows the

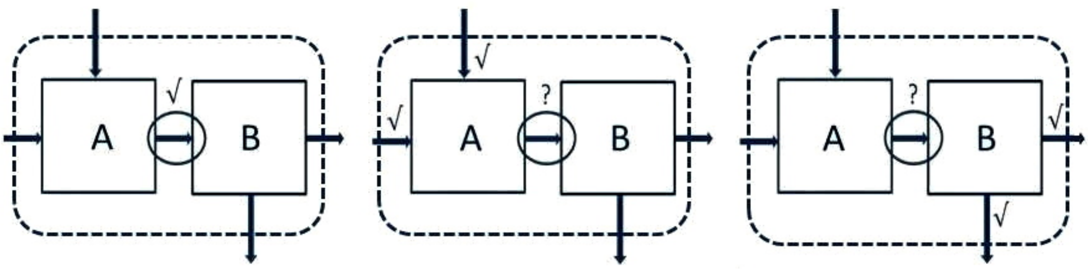


Figure 2.3: Calculation of the membership functions belonging to an internal flow [Source: I]

calculation of the membership functions belonging to an internal flow. On the left, the input data membership function is calculated. The other pictures show the functions resulting from the two balance constraints by assuming the internal flows to be unknown and by using fuzzy input intervals for the external flows. In the second example (Figure

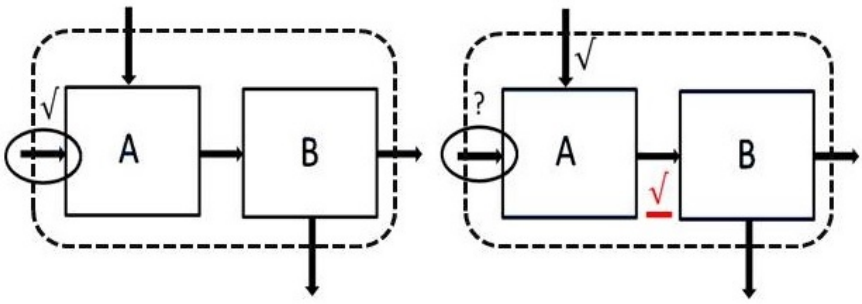


Figure 2.4: Calculation of the membership functions belonging to an external flow [Source: I]

2.4), the membership functions of an external flow are given. The left one is the input data membership function and the right one is resulting out of the balance constraint. To calculate this constraint function, the internal flow, which is calculated in advance, is used, while the remaining external flow functions that are used are based on input data.

2.2.5 Alternative approaches on uncertainty characterization

Uncertainty estimates remain subjective to some degree and thus, reconciled fuzzy ranges could be wrong even though flow data and balance constraints are in perfect agreement with a high degree of consistency. Being over-confident results in low consistency levels and small fuzzy ranges, while being over-conservative results in high consistency levels at the cost of large ranges (cf. Laner et al. 2015). In order to illustrate the trade-off between uncertainty ranges and consistencies, two alternative approaches on data characterization are proposed. In the first case, the uncertainty factors are reduced, which means more confidence in the data sources. In the second case, the treatment of overdetermination of flows is modified by using a conjunctive approach on data fusion. Only values that are in the uncertainty range of any source are considered (cf. Destercke 2014). The second case gives also higher weight to the actual data sources and is useful in identifying problematic data efficiently (through high conflict in the input data).

2.3 The significance of global sensitivity analysis - a guidance for the appropriate usage of sensitivity analysis in dynamic MFA

This chapter is based on Article II: "Evaluating the Use of Global Sensitivity Analysis in Dynamic MFA" by Džubur et al. (2016). Detailed information can be found in the article in the appendix.
In contrast to static MFA, where material flows are determined for one balancing period and are therefore time independent, material stocks and flows in a dynamic material flow model can potentially depend on all previous states of the system (Baccini and Bader, 1996). Dynamic MFA has recently become increasingly popular, with a primary focus on the investigation of material stocks in society and associated EOL flows (cf. Laner and Rechberger, 2016). Metals in particular have been subject to dynamic MFA because of the large accumulated metal stocks in society and their potential value for society as secondary raw materials (cf. Chen and Graedel 2012; Müller et al. 2014). Sensitivity analysis is carried out to investigate the effect of individual assumptions and parameter specifications on the model output by exploring the effects of the changes of input parameters on the model output. Whereas local sensitivity analysis methods focus on testing different perturbations of constant or uncertain input parameters and analyze the specific consequences in the output, global sensitivity analysis focuses on the uncertainty in the output and how it can be apportioned to different sources of uncertainty in the inputs (Saltelli et al. 2008). The process of recalculating outcomes under alternative assumptions to determine the impact of variables using global sensitivity analysis can be useful to identify model inputs that cause significant uncertainty in the output in order to increase robustness of the model and understanding of the relationships between input and output variables (Pannell 1997). Analytical local methods using partial derivatives are usually not useful in dynamic MFA systems, given that the model input parameters are uncertain and the model is of unknown linearity. Derivatives are only informative in the base point where they are computed and do not provide for an exploration of the rest of the space of input factors, which does not matter for linear systems, but greatly matters for nonlinear ones (Saltelli et al. 2008). Moreover, the global method of regression analysis is typically not a useful option in this context, given that it describes only the fraction of linearity within the model output and remains ignorant of the rest of uncertainty or variance within the model (Saltelli et al. 2008). The usual treatment of dynamic MFA in previous literature is local, using one-at-a-time (OAT) analysis, where

one input variable is changed whereas the others remain fixed in order to see what effect this produces on the output (Murphy et al. 2004, see also chapter 1.3.2). However, this method is very time-consuming if the system consists of many inputs, which need to be observed. Besides, because materials typically reside for some time in the use-phase, input parameters of previous periods affect the uncertainty of the output (in use stocks, old scrap generation) in later periods. Such time-delay effects are important if model parameters vary over time, which may often be the case in reality (e.g., the share of a material used in a specific application may not be constant over time, but vary because of technological, legal, or socioeconomic changes). Further, OAT analysis cannot account for the combined effects of parameter changes such that interaction effects attributed to the simultaneous variation of parameters are ignored. Bader et al. (2011) used a kind of global analysis to investigate a copper flow model for Switzerland by focusing on specific stock saturation-based scenarios, and McMillan et al. (2010) used the Fourier amplitude sensitivity test for global sensitivity analysis (cf. chapter 1.3.2). Buchner et al. (2015) explored the variations in the total scrap output of Austrian aluminum stocks and flows by applying global sensitivity analysis for main effects using the effective algorithm for computing global sensitivity indices (EASI by Plischke 2010). The analysis focused on the decomposition of the output variance with regard to parts attributable to stochastic input variables and showed that only small parts of the total output variance could be explained by the variation of single parameters in the same year. Therefore, it was the aim of this study to provide guidance on how to conduct sensitivity analysis in dynamic MFA with regard to how the interaction effects (attributed to simultaneous change of several parameters) influence model results, how the time-delay effects (influence of parameter values from previous periods on results of subsequent periods) influence model results, and to find problem- and model-specific recommendations concerning sensitivity analysis in dynamic MFA. Thereto, the state of the art of sensitivity analysis in dynamic MFAs is reviewed and novel applications of sensitivity analysis are explored. An archetypal dynamic material flow model is established as a highly simplified, reduced version of the national aluminum flow model presented by Buchner et al. (2015) and investigated using a sample-based approach of variance-based global sensitivity analysis. The model contains the essential elements of input-driven top-down dynamic material flow models, which are the distribution of produced materials into different use sectors and the lifetime of products (i.e., in use stocks) in these sectors (cf. Müller et al. 2014). Based on the analyses, recommendations concerning the choice of sensitivity analysis methods for dynamic MFA are provided.

2.3.1 Case study

The developed archetypal model is a reduced model based on existing dynamic material flow models for metals (Buchner et al. 2015, Pauliuk et al. 2013, Liu and Müller 2013) focusing on the core elements of dynamic MFA, namely, the use-phase and associated material stocks and EOL flows. The stocks and flows are modeled using an input-driven, top-down approach. Consequently, the pre-defined material input is distributed to three sectors with different residence times, defined through Weibull functions, which are widely used to express product lifetimes or failure rates of material components (cf. comparison of lifetime distributions in dynamic MFA by Melo 1999). The sector split ratios of materials and average lifetimes are uncertain and expressed as independent normally distributed variables. The model output is old scrap, consisting of three outputs from the three sectors of materials in stock. The model output for each time period t is obtained by the following convolution formula:

$$O(t) = \sum_{i=1}^{3} O_i(t) = \sum_{i=1}^{3}\sum_{\tau=1}^{t} r_i(\tau) l_i(t-\tau) I(\tau) d\tau \qquad t = \{1, 2, ..., T\} \tag{2.7}$$

In Equation 2.7, T denotes the time range of the system observation, $I(t)$ denotes the input in the period t; $r_1(t), r_2(t)$ and $r_3(t)$ the three sector split ratios in period t, with the corresponding average lifetimes $l_1(t), l_2(t)$ and $l_3(t)$. τ is the time the material input enters the specific sector, taking values between 1 and t. A schematic illustration is given in Figure 2.5. The mean values of the sector-specific average lifetime probability density functions are denoted as m_{l1}, m_{l2}, m_{l3}. The variance in the old scrap is an aggregation of the variances of the uncertainty within input parameters. The reduced model is subsequently used to study how the total variance of the old scrap output can be properly apportioned to the uncertainty of the varying input parameters over time and which changes in input parameters affect the variance of output most in which time period.

2.3.2 Observed scenarios

Different model setups (=scenarios) are used to analyze interaction and time-delay effects on the model output. In the first scenario, the counteracting effects of lifetime and sector split ratio are explained by the means of the sector output O_2 over time. The effects of changes of time-independent parameters are explored. Because of the residence time, the inputs enter the output sectors with delay and the changes in those parameters can affect the output at any later time given that the time of outflow is random. This

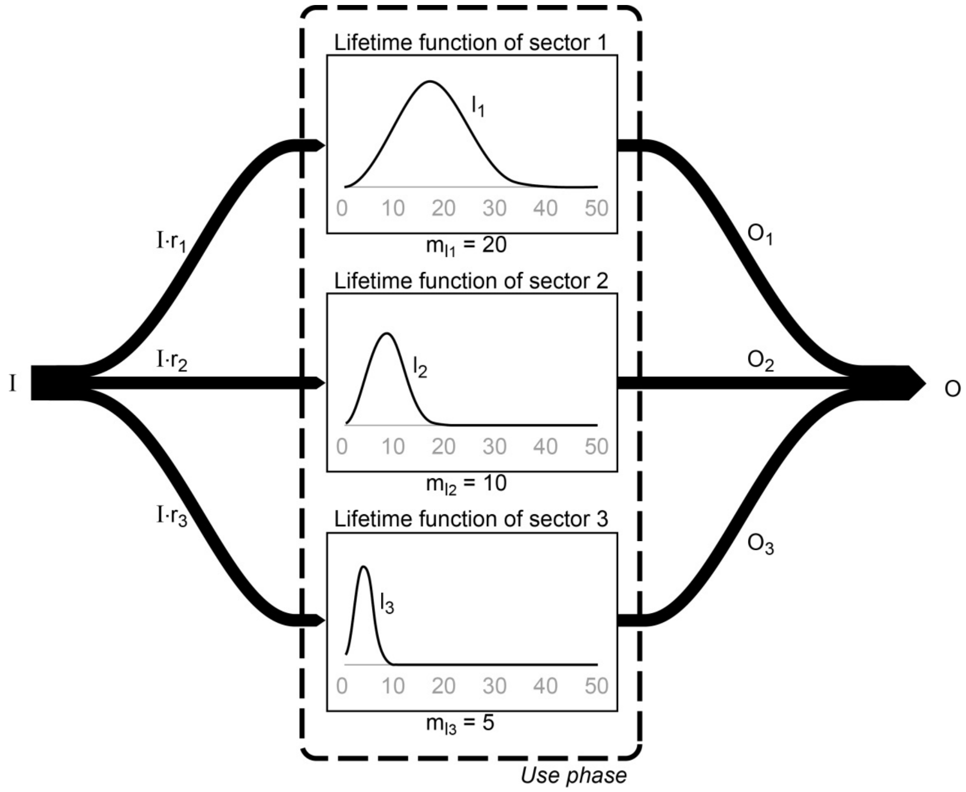


Figure 2.5: Reduced dynamic material flow model [Source: II]

scenario is important to understand the further ones. In a second scenario, the system is tested for different inputs as a model driver, a constant and a linearly growing input (which is similar to the aluminum input in Buchner et al. 2015).

A third scenario focuses on the effects of time-dependent parameters. In this case, effects of parameter variation on the output are accumulated and it is not possible to trace the individual contribution of input parameters from specific previous years to the output in a certain year. Therefore, in this scenario, the sensitivity of output in a specific year with respect to time-dependent parameters is investigated. This represents the frequently occurring situation in dynamic material flow modeling when current in use stocks and old scrap flows are calculated from historical data. In order to compare time-varying with stationary parameters, the parameters were defined to change step-wise for three time periods. A practical example of the first sector with rising mean ratio m_{r1} and simultaneously rising lifetime m_{l1} would be the aluminum use in vehicles (cf. Buchner et al. 2015).

2.3.3 Global sensitivity analysis

Variance-based sensitivity analysis is used to find out how the variance of the output over time can be decomposed into the conditional variances caused by the input parameters from current and previous periods. The interest is not only in single, but also interaction effects caused by combined effects of parameters $p_1, ..., p_K$ on the output $Y = f(p_1, ..., p_K)$. The total variance of the output $V(Y)$ is an aggregated sum of all conditional variances of the output. It can be restricted to one, or a combination of several parameters. The normalized partitions are denoted as sensitivity indices. Three kinds are considered (see also Saltelli et al. 2008, chapter 4) ($i = 1, .., n$):
First order effect of parameter i:

$$S_i = \frac{V(Y\Big|p_i)}{V(Y)} \tag{2.8}$$

Total order effect of parameter i:

$$S_{T_i} = 1 - \frac{V(Y\Big|p_{\sim i})}{V(Y)} \tag{2.9}$$

Higher order effect of parameter i:

$$S_{H_i} = S_{T_i} - S_i \tag{2.10}$$

$V(E(Y\Big|p_i)$ is the expected reduction in variance by fixing p_i, and $E(V\Big|p_{\sim i})$ is the expected variance by fixing all parameters but p_i. The first order effect S_i is the impact on the variance of the output of a parameter alone, whereas the higher order effect S_{H_i} gives all combined effects of a parameter with other parameters, and the total order effect S_{T_i} is all kinds of impact on the output's variance caused by a parameter, alone and in combination with other parameters. As the conditional variances are normalized, the sum of S_i is smaller in general and equal to 1 if there are no interactions in the model. In this special case, $S_{H_i} = 0$, so that S_{T_i} is also 1. S_{T_i} is in general greater than 1 (because interactions are counted multiple times).
The calculation results of these effects are obtained faster by a short-cut method than one by one. This method uses a sample-based approach and is based on procedures by Saltelli et al. (2008, chapter 4). Matrices are used to fix parameters or groups of parameters while the rest of parameters is random in order to calculate $V(E(Y\Big|p_i)$, $E(V\Big|p_{\sim i})$. Monte Carlo sampling is used to calculate the results. To evaluate the plausi-

bility of first-order indices and to test their convergence, the results of the sample-based approach are checked against first order indices derived using a variance decomposition method based on Fourier Transformations, namely the EASI algorithm (Plischke 2010). Such algorithms are suitable to determine main parameter effects computationally more efficient than the sample based approach described above.

2.4 An evaluation on modeling structures for dynamic studies of building stocks on a goods and substance level

This chapter is based on Article III: "Evaluation of modeling approaches to determine end-of-life flows associated with buildings: a Viennese show case on wood and contaminants" by Džubur et al. under revision. Detailed information can be found in the article in the appendix.

The longevity of buildings and thus, the long residence time of their potential resources in stock may lead to an aggregation of contaminants in the stock, which may pose quality constraints for future recycling activities (Brunner 2010; Pivnenko et al. 2016). Various dynamic MFA studies on C&D (construction and demolition) waste of the building sector have been published in the past decade. Dynamic bottom-up studies were presented by Lichtensteiger and Baccini (2008) and Tanikawa et al. (2015). A model on the analysis of waste wood streams from buildings using a top-down approach was published by Müller et al. (2004) which had its focus on the Swiss lowland. In the study of Müller et al. (2006), the focus was on the dynamics of the building stock of the Netherlands, analyzing and calibrating the stock with regard to the major drivers, such as population, lifestyle (floor area per person) and material intensity. The aim was to give a future prognosis by observing scenarios. Bergsdal et al. (2007), Sartori et al. (2008), Brattebø et al. (2009), Sandberg et al. (2014), and Hu et al. (2010a, 2010b) adapted this model. Based on the same idea, Pauliuk et al. (2013) propose a novel dynamic stock model with an optimization routine to identify and priorize buildings with the highest saving potentials. Further top-down studies are given by Huang et al. (2012), using estimations of long-term material demand, and Gallardo et al. (2014), using a leaching approach to observe the vulnerability of building stocks to earthquakes. The dynamics of building stocks, and therefore also dynamics of aggregations of contaminants, are hard to analyze since data is scarce on the input side and mostly a result of estimations not only on the substance but also on the goods level (Kohler and Hassler, 2002). Thus, uncertainties arise not only on the goods level and on the substance level, but they are associated with the driving input parameters, such as the inflow to the use-phase and the duration in use, making the model structure uncertain. Beside the uncertainty caused by the diversity of residential structures and building types as well as their material contents, lifetimes of buildings vary strongly and are therefore hard to determine. Furthermore, there are only few material flow studies on stock dynamics on the goods together with the substance level by now. Studies on comparing stock models on the substance level have been published by van der Voet et al. (2002) and Kleijn et al. (2000). Both studies compare a delay approach based on lifetime considerations of the input to a leaching approach based on a leaching share of the stock. Van der Voet et al. (2002) present analytical conditions under which the calculations of the leaching approach will produce acceptable solutions for dynamic models which should typically be solved using the delay approach. This study was built on these two archetypal modeling approaches and extended them to more accurate models for EOL wood flows associated with buildings in Vienna. In the delay approach, EOL wood flows and contained contaminants (lead, chlorine, and polycyclic aromatic hydrocarbons (PAH)) are determined based on past wood inputs and product lifetimes (i.e. residence time of wood constructions in use). In the leaching approach, bottom-up estimates of the wood stock in buildings at different times are combined with estimates of demolition and renovation rates to calculate the output of wood and contaminants from the use-phase. Using the case of wood stocks and EOL wood flows of Viennese buildings, these two modeling approaches are compared in the present study. The goal is to investigate the data requirements of each approach and the effects of inherent modeling assumptions on the resulting stocks and flows of wood and therein contained contaminants.

2.4.1 Case study

The proposed case study for the dynamic material flow model is the wood stock in Viennese buildings together with its demolition activities (investigated in a GIS-based analysis by Kleemann et al. 2016). The variables of interest are on the one hand, the amount of EOL wood flows resulting from demolition and renovation activities of buildings, including beams in wood (roofs, ceilings) and wood extension products (windows, doors, floors and others). On the other hand, the substance level is considered with respect to the quality of wood flows regarding contaminants and impurities (lead, chlorine, PAH). These contaminants are chosen as they have been observed at elevated levels in waste wood collected for recycling, i.e. directed towards particle board production

(BMLFUW 2012). The sources of the contamination are wood preservatives on the one hand, which were used in the past (and are nowadays forbidden), and coatings and adhering particles on the other. As the amount of wood in buildings is strongly correlated to the construction period (Kleemann et al. 2016), the amounts of wood as model input parameters are classified according to the construction period of the respective building. Moreover, as all contaminants have been used in applications which were forbidden in the course of time, the substance flow variables depend on time. The model is used to estimate the amount of EOL wood flows, and lead, chlorine and PAH in EOL wood flows from demolition and renovation activities in Vienna over time employing all available information on the flows and stocks of wood in the building sector.

2.4.2 Data assessment and uncertainty analysis

Uncertainty levels are assigned to the data based on the method suggested by Hedbrant and Sörme (2001). The same four levels are assumed as in the first study and the uncertainty range d is calculated in the same way (see chapter 2.2.2). The data is fed into the model, where all variables are assumed to be normally distributed. Resulting of the underlying uncertainty function, standard deviations for the density functions are derived, whereby the standard deviations correspond to the uncertainty ranges.
In a first step, these normal distributions are assigned to the input data. Monte Carlo simulation to calculate the output cannot be done for each parameter separately. Therefore, the probability density functions of the types of wood categories are calculated in advance by multiplying the wood in stock for each year with the wood content according to the age class of the building, and dividing it into the six types (the categorization of age classes in the building stock needs to be considered, too, in the leaching approach). As the product of normally distributed variables is not normally distributed, a normally distributed approximation by Ware and Lad (2003) is considered as the probability density function of the resulting shares of types of products. Then, Monte Carlo simulations to calculate the output flows are performed on these shares, on the lead, chlorine and PAH values per wood category and on the technical lifetimes in the delay model.

2.4.3 Comparison of model approaches

It should be emphasized that the stylized models of wood stocks and flows are used to investigate the effect of differences in the modeling approaches on the outputs, rather than to give a highly realistic picture of the Viennese situation. This is outside of the scope of the study, as more elaborate data mining and additional information on key input parameters would be required. Because demolitions of buildings are mainly carried out when they are planned to be replaced by new buildings, and as both, demolitions and renovations of buildings, are cost-intensive, it is assumed that the actual output of EOL wood is externally influenced by the business cycle. Thus, the higher the turnover of the building industry, the more is demolished and renovated, and the rest remains in a pool of "depleted buildings" of the stock, which represents a hibernating stock in both models. While the leaching approach reflects the actual economic situation (provided real-time data is available), meaning that the business cycle has a direct influence on the rate of renovations and demolitions in a specific year, the delay approach is lifetime-based, meaning that only a very small percentage of buildings at the end of their lifetimes is assumed to depend on the business cycle (in order to enable extensions of lifetimes). Because PAH and lead coatings were banned in the middle of the 90s (ChemG. 1996; cf. RIS 2016) and chlorine components have been increasingly replaced since then, it is assumed that input from demolition wood of wood products from the middle of the 90s (1998-) on is free of those contaminants. In order to extend the models to predict the future development of building EOL wood flows and contaminants, the building stock is assumed to rise annually starting from the last year of observation. Based on the predictions of a growing population in Vienna (Statistics Austria 2014a), and on the average number of buildings per 1000 inhabitants (Statistics Austria 2014b) (assuming a constant per capita floor area (cf. also Statistics Austria 2014b)), the assumed growth of the building stock is 0.38% annually.

Leaching stock approach

Every stock is classified into age categories. The output O (in tonnes of wood) is then calculated as a leaching part of the stock for each year t, thus,

$$O(t) = f(t, c + r) \cdot S(t), \tag{2.11}$$

whereby f is the sine function of the business cycle that depends on the mean value $c+r$ of the stock (the sum is constant over time), c is the demolition and r the renovation rate, and S the stock of building wood.

Delayed input approach

This model builds on the knowledge of newly built buildings within each decade since 1950. There is no data provided for this input. The change in stock is the net growth of the number of buildings in Vienna. The input is the sum of the net growth and the overall output of each building period, which is determined through the age categories of the stock in each period. The evolution of the initial stock (built up before 1950) is estimated by the classification of age categories of the stock. The amount of wood in the stock is determined based on the wood content of each product category in each construction period. The products within a period are assigned the associated technical lifetimes. The output O_i of waste wood of each product category i ($i = 1, .., 6$) is calculated as a delayed share of input in each year t, which depends partly on the business cycle. As the major part of Vienna's building stock is inhabited or in use, there is a high turnover of constructions and renovations, and therefore, a need for replacement at the end of the technical lifetimes. Thus, the variable p, which represents the share that is not influenced by the business cycle, is assumed to be 99%. The output of a construction product category is

$$O_i(t) = pI_i(t - L_i) + f(t, 1 - p)I_i(t - L_i), \tag{2.12}$$

whereby f is the same sine function as in the leaching approach with a mean value of $1 - p$, I_i is the amount of wood of product i going into the stock, and L_i is the product lifetime following a Weibull distribution (with a normally distributed mean value). The overall output is

$$O(t) = \sum_{i=1}^{6} O_i(t) \qquad \forall\, t. \tag{2.13}$$

The comparison of the approaches is not only done on output flows but also on the stocks in order to analyze the differences in amounts, and therefore, the differences within the approaches in full. The substance level is calculated by multiplying the wood products with the respective substance concentrations in both approaches.

2.4.4 Cross-checking of model results

The results of the modeling approaches are cross-checked with independent estimates in order to get an impression on how well the model outputs fit reported data. The amount of waste wood is estimated based on the total amount of demolition wood in Austria (BMLFUW 2013) taken on a per-capita share for Vienna (UN data 2013). On the substance level, representative contents of lead, chlorine and PAH are derived from a study on waste wood flows in Switzerland (BUWAL 2004). These estimates are quite uncertain, as the taken samples vary strongly for each wood product category.

2.4.5 Sensitivity analysis

Sensitivity analysis is used for the identification of critical parameters, whose variation has the largest effect on the variation of the model results. This increases the understanding of the relationships between in- and output variables of a model. The model outputs are analyzed for a) the impact of specific parameter perturbation (local sensitivity analysis) and b) the overall distribution of the uncertainty of the output (global sensitivity analysis, cf. Article II, chapter 2.3).

Local sensitivity analysis is performed on the critical parameters of both approaches, which are the technical lifetimes and the demolition and renovation rate. Furthermore, as part of the initial stock from before 1918 has far the highest wood content and therefore plays a major role in both modeling approaches, and as this part of the initial stock's actual magnitude is highly uncertain, scenarios are tested for the reallocation of amounts of this building stock to later building periods. Other parameters which were tested are the shares of specific building periods on their influence on the EOL substance flows of PAH in order to find out which period influences recent outputs the most.

Global sensitivity was analyzed for the first order effects (without interactions with other parameters) of the model output (EOL wood flows, substance flows) using the EASI algorithm (cf. Plischke 2010). This was done for all parameters in a first step. In a next step, the output flows (on the goods level) were also analyzed for bundled groups of parameters used as input parameters (the shares of wood categories) which enter the stock in each year.

3 Results and Discussion

The results and major findings of the three investigations on studies are presented and discussed in the following three sections.

3.1 Fuzzy-set based data reconciliation

3.1.1 Results

The reconciliation algorithm is applied to determine the flows of the Austrian wood balance system. As a result of the data reconciliation procedure, the reconciled fuzzy sets, indicating the possible range, and the consistency levels, indicating the agreement between the given data and the mass balance constraints, are determined for each flow in the model. The results are compared among the three approaches to characterize the input data taking the reconciled ranges and the achieved consistency levels into consideration.

Comparison of consistency levels and reconciled fuzzy ranges

The result of the initial approach (=base case) is given in Figure 3.1. The reconciled fuzzy ranges of each flow are marked in the trapezoids. The core is listed in the upper part and the support in the lower part of each trapezoid. The de-fuzzified value (arithmetic mean of the core in this case) defines the thickness of the flows, and the color scale denotes the consistency level for each flow (grey flows are calculation results). The results of the alternative data characterization approaches are depicted in Figure 3.2 (reduced ranges) and Figure 3.3 (intersected data). The color scale highlights that the consistency levels decline for both alternative approaches, consistently for the reduced ranges and with less discrepancy for the intersected data approach (with exception of the intersected flows f19 (semi-finished products for the building industry), f4 (and sawmill by-products for pellets), which have the lowest consistency levels).

All flows related to only one process are linearly dependent and share the same level of consistency (as indicated by the colors in the figures). The high consistency levels in

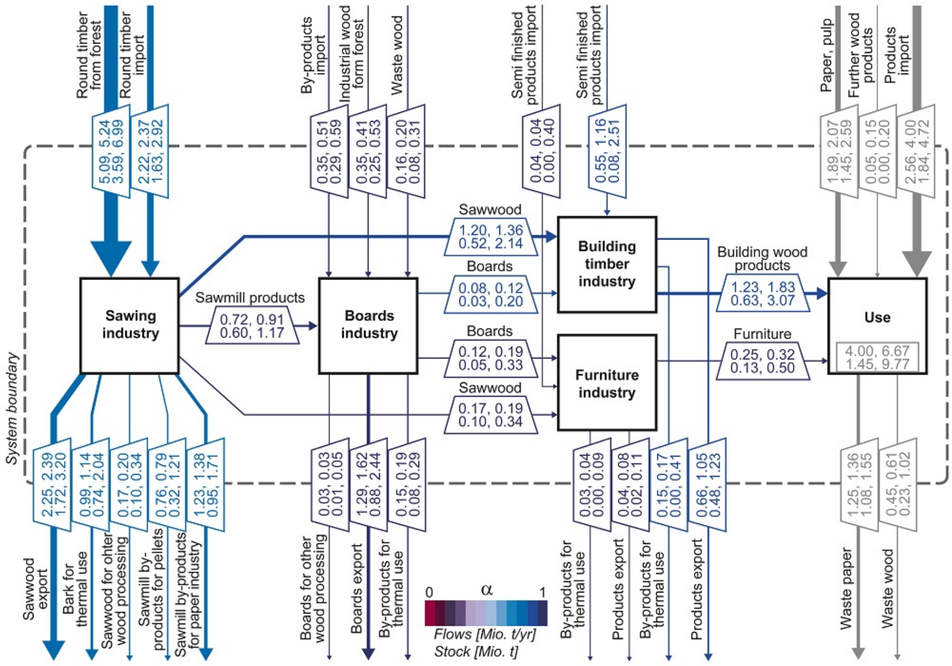


Figure 3.1: Reconciled wood flow model [Source: I]

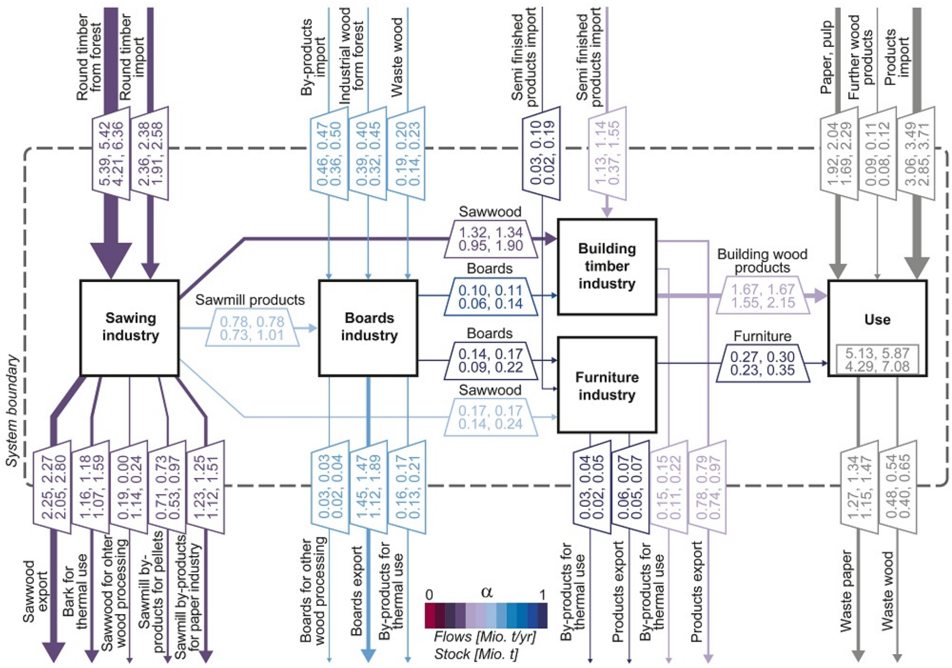


Figure 3.2: Reduced ranges [Source: I]

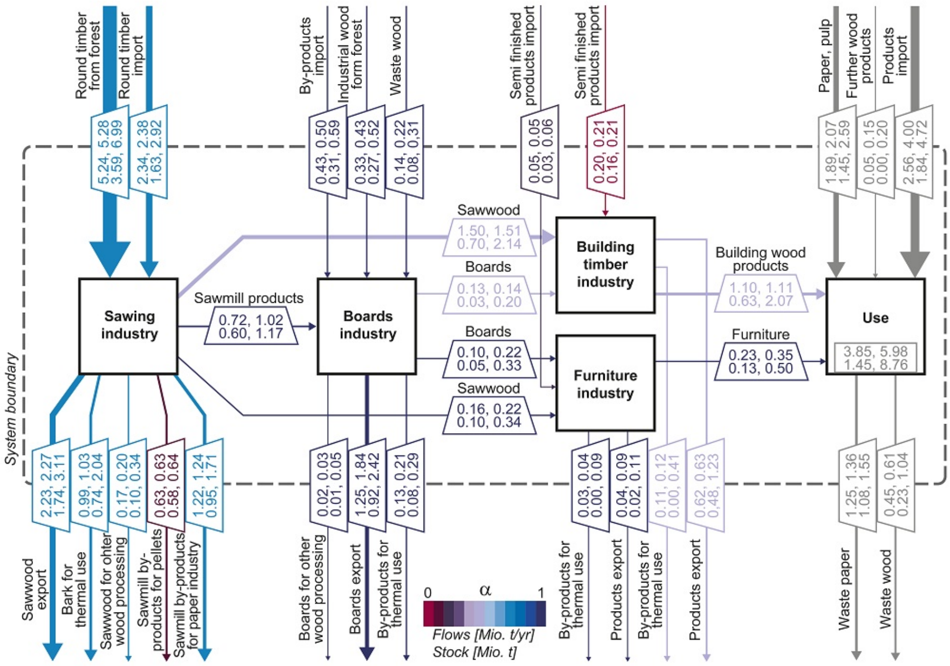


Figure 3.3: Intersected data [Source: I]

the base case indicate a good agreement between the fuzzy ranges. Reducing the ranges causes a reduction of the consistency levels of approximately 24% of the sawing industry process and 19% for the building industry process (the ones with the lowest consistency levels). Comparing the intersected data approach to the base case, there is only a significant change for the building industry, with a 20% lower consistency level. This is due to the fact that the changes in the reconciliation steps are only caused by narrower fuzzy intervals of the overdetermined intersected data (which have the lowest consistency levels by far). This confirms a trade-off between the uncertainty characterization and the consistency levels, because the levels decrease when more trust is given to the input data.

Comparing the figures, it can also be observed that each approach gives slightly different results for the reconciled fuzzy ranges. The fused data points lead to enlarged fuzzy input intervals in the base case and in the reduced ranges approach, which leaves a margin for the balance constraints. The reconciled ranges of f19 (the building industry flow), and f4 (the sawmill by-products flow for pellets), are increasing for the base case and reduced ranges, but decreasing for the intersected data approach. The diverse effects in the intersected data approach are caused by the uncertainty characterization for overdetermined flows with heterogenous conversion factors and commodity distributions.

Detection of weaknesses

In contrast to all other flows, the fuzzy ranges for the semi-finished products for the building industry (f19) are greatly different for all approaches. It is also the flow with the lowest consistency level in the intersected data approach. This is caused by the high conflict in input data. The values of the two transformed data points of this flow are so far off each other that at least one of them must be substantially flawed. It is difficult to identify which one, as the uncertainty factors for both data points are relatively high. Therefore, f19 is treated as a free variable in a next reconciliation step (see Article I) in order to get a better understanding of the magnitude of the flow. The data point which is closer to the de-fuzzified value of the result is chosen as only data point, and the reconciliation is iterated by ignoring the other data point in the uncertainty characterization. Thus, the consistency level of the building industry is raised to 1, indicating perfect agreement.

3.1.2 Discussion

Reconciliation algorithm

The fact that the output of the developed approach contains not only the reconciled flows and their resulting uncertainty, but also information about their consistency within the model, is the main added value of the developed approach in contrast to other reconciliation methods. A recommendation for consistency level benchmarks is given in Table 3.1. This indicates the agreement of the data for a flow within the model. α-levels above 0.9 stand for excellent agreement. It is assumed that α-levels above 0.5 are acceptable while all values below indicate poor agreement. In the latter case, the data (or the model) is in need of an update.

The existing Linear programming method for reconciliation under fuzzy constraints

Table 3.1: Recommendation for consistency level benchmarks [Source: I]

α	agreement
>0.9	excellent
>0.7	good
>0.5	fair
0.5-0	poor

from literature (Dubois et al. 2014, Laner et al. 2015) is only applicable to membership functions of triangular or trapezoidal shape. However, as most of the flows result from multiplications with conversion factors or commodity distributions, the resulting membership functions are rather of a curved shape. Thus, using a linear program, the results are inaccurate, as the intersection points may be shifted. This can lead to big deviations of membership functions through error propagation (cf. Laner et al. 2015). The generalization to common membership functions is a main innovation of the developed approach. In the resolution of this study, precision up to the second digit after the comma can be expected.

Effect of uncertainty characterization

How can a system with no or poor agreement be updated to get a feasible solution or a solution with higher consistencies? The conflict may appear through uncertainty ranges which are defined too narrow. If a very low level of consistency cannot be increased by an appropriate enlargement of uncertainty ranges, the first step should be a check of input data for potentially erroneous data sources related to the problematic flows or processes respectively. Full reliability of the model is assumed, since the constraints are fixed and not uncertain. If it is not possible to improve the input data in order to rise the consistency level in an appropriate way, the balance system (i.e. the model) should be critically reconsidered with respect to correctness and completeness. This iterative way of improving data and model is typical for the procedure of doing an MFA (cf. Brunner and Rechberger 2004, Laner et al. 2014).

The trade-off between uncertainty ranges and consistency levels provides a better understanding of the way the data should be characterized. The highly conservative characterization of uncertainty in the base case leads to large ranges and excellent consistencies which is not really representative if the data quality is considered. Besides, the scope of the flow ranges leaves a lot of margin in the reconciliation process. In the present case study on Austrian wood flows, the preferred uncertainty characterization approach is the reduced ranges approach. While all fuzzy ranges become more precise, the loss in consistency is modest compared to the base case.

Larger, more complicated balance systems with similar data quality assessments should be treated by using the base case. The intersection method points out the weaknesses within the wood flow system. The lowest degree of consistency is almost zero, which means that the wood flow model is untenable and in need for changes. In the case of f19, no update of the system leads to reconciled ranges close to the value obtained by ignoring the variable. As relatively many overdetermined flows are faced for these (and especially also larger) wood flow systems, this approach would require a lot of rework to obtain acceptable consistencies according to Table 3.1. This is not worthwhile, as the gain in information through the reconciled values of this method is not so high.

Comparison to existing fuzzy-based reconciliation approaches

In order to validate the model, it was cross-checked using a linear uncertainty characterization with the leximin approach using fuzzy linear programming by Dubois et al. (2014). The application on the Australian copper system, overtaken from van Beers, van Berkel and Graedel 2005, allows the usage of the linear program as each of the flows is uniformly defined by a triangular membership function. Except for some differences in the system's assumptions, it was possible to reproduce the results of the leximin approach with the presented algorithm. It should be clarified again that linear programming is only applicable to such simple cases with triangular or trapezoidal membership functions, and leads to imprecise results if multiplications are considered. In such cases, a generalized approach, as the one presented here, is needed. Besides, the iterations of reconciliation in the leximin approach are very time consuming (flows with lowest consistencies are always fixed in each iteration step during the reconciliation process). The reconciliation method presented in this study offers a more practical approach, since it consists of only two reconciliation steps. As the internal flows are attached to all processes and therefore their reconciliation affects all other flows in the next step, it is natural to reconcile them in the first step.

3.2 Global sensitivity analysis

3.2.1 Results

The results are analyzed for the three distinct model setups, presenting the major findings with regard to the importance of lifetime and sector split ratio for a single output, multiple outputs (=total output) and the consideration of time-varying parameters. Each scenario is tested with regard to time-delayed and interaction effects.

Importance of lifetime and sector split ratio on a single output

The relationship between the sector split ratio of the output and its lifetime follow the same patterns for the first and the total order indices for each sector: the effects are reverse. The duration of the growth period, the saturation period and the degeneration period of the output are influenced by the mean value of the average lifetime, while the sector split ratio is responsible for the amount of output. As long as the flow volume is increasing and the in use stocks are growing (growth period), the uncertainty in average lifetimes is more important than in situations where in use stocks are closer to saturation or decreasing, and EOL flows also follow a decreasing trend (saturation period). For the latter kind of situations, the uncertainty associated with sector-split ratios comes to the fore. The higher order indices become smaller with an increasing number of Monte Carlo samples and are negligible at 100,000 sampling runs. The results of the first order effects are compared to results obtained by using the EASI algorithm, which are almost identical, validating that there are no higher effects.

Sensitivity Analysis of the total output

The dynamic system was tested for a constant input and a linearly increasing input over time. The latter has been chosen to resemble typical trends in metal consumption in industrialized countries and is exemplarily based on the increase of aluminum consumption in Austria (see Buchner et al. 2015). Figure 3.4 denotes the curve progression of these inputs, the corresponding outputs and sensitivity indices. The constant case shows that all lifetimes are influent in the unstable phase of introduction and the sector split ratios are influent in the stable phase when the output is saturated. The same holds for linearly increasing input, the influencing parameters are the mean average values of lifetimes in the introduction phase and the mean values of the sector split ratios in the saturation phase. The introduction phase is the period of non-linear behavior of output, thus, the function derivative of the output is growing. The saturation phase is the period where the rate between output and input is practically constant; here, the function derivative of the output is also constant. While effects overlap during the constant input case, the annually growing input and, consequently, also growing output stretches the effects over time.
The higher order indices are small but still present after 300,000 Monte Carlo runs. As we know that the single output in the previous scenario has no higher order effects and the outputs are independent, this means that the higher order effects converge towards zero for each case. This is again validated by the EASI algorithm which shows that there are no significant higher order effects.

Parameter effects on the output of a specific year

The first order effects show again the same behavior as the total order effects for both time-varying and stationary parameters. The higher order effects converge to zero with an increasing number of simulation runs. The effects are tested for the output at the end of the observation period (year 50). Obviously, the effects of the sector-split ratios of sectors with shorter lifetimes appear close to the year of output 50, whereas the

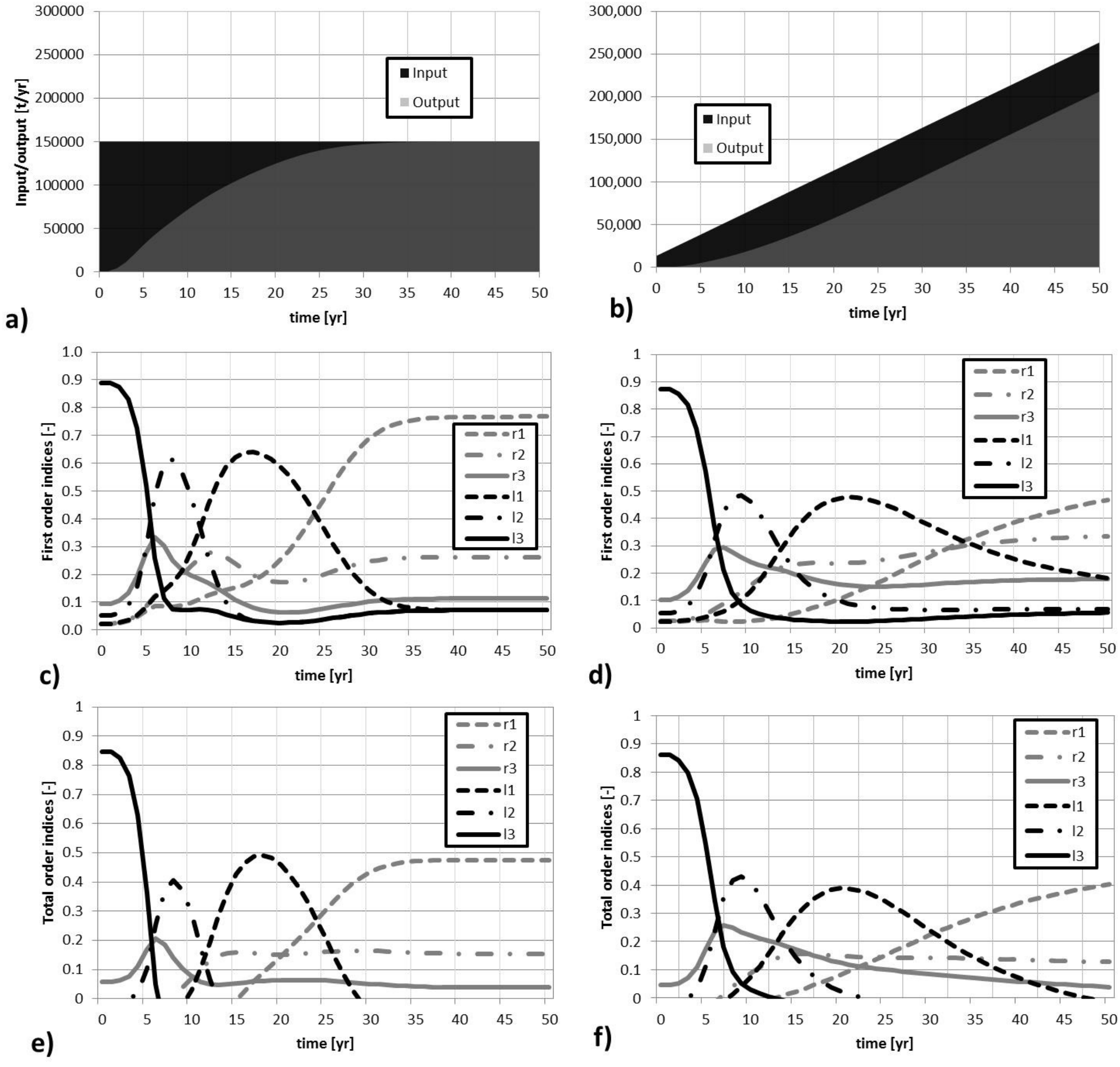


Figure 3.4: Sensitivity indices for a constant and a linear input [Source: II]

parameters related to outputs in earlier modeling periods are more important for the output of year 50. The shorter the lifetime, the higher is the concentrated effect in one period. The changes of parameters over time affect the behavior of sensitivities and lead to nonlinear effects in output dynamics.

3.2.2 Discussion

Reduced dynamic material flow model

The computational effort required of this variance based method to detect such sensitivity indices is very high, especially if the parameters are observed over a long period of time. This analysis indicates that in such general dynamic MFA cases of combinations of sector split ratios and lifetime functions, higher order indices are not expected to be significant and can be neglected. Therefore, in these cases more efficient algorithms analyzing first order effects, such as the EASI algorithm, can be used, and large numbers of input parameters (like time variations of parameters for each year in this example) can easily be dealt with. However, there are specific circumstances, when higher order effects may become relevant for sensitivity analysis in dynamic MFA. For instance, this could be the case for very small material flows, which are distributed into more flows at a later stage of the model. An example would be the material flow out of a very small use sector, which is subsequently directed to a sorting and upgrading plant producing secondary raw materials. Higher order effects may be relevant for this secondary raw material flow because the probability density function for the respective sector split is located close to zero, and several other parameters are multiplied with the sector split ratio to calculate the flow of interest. In general, significant parameter interaction effects on the model output may be expected if the output is the product of several variables, and (at least) one of the variables is defined in a way that zero lies within the set of probable parameter realizations. It holds that the more often zero is attained within the set of outcomes of the final output, the higher the interaction effects. A similar relationship may be given for emission flows with low emission factors. In classical cases, when the observed model output is not a product of many factors with at least one frequently taking zero values, the variation of the output can be explained through the first order effects over time.

Due to the use (duration) of products the effects of parameters related to inputs to the use-phase have a delayed effect on the EOL flows and therefore the sensitivity indices of the parameter values also need to be considered with regard to the delay. In most cases the modeler is interested in finding out which parameters affect the model output for a specific year (e.g. current in use stocks or old scrap generation). For time-varying parameters it holds that every change of their probability density function (in our example, the mean value) needs to be considered as a new variable. Here, the appearance of the effects of a sector split ratio and the corresponding lifetime can be approximated by subtracting the average lifetime of the year of observed output. Thus, for short average lifetimes it holds that the sector split ratios and their corresponding average lifetimes can be neglected in early periods, while for very long lifetimes, the sector split ratios and their corresponding lifetimes are practically negligible in the years close to the output. Thus, the number of parameters can be reduced to potentially important ones. Otherwise, for instance in the case of annually changing parameter values, the computational cost of the sample based approach for sensitivity analysis could become very high. The comparison of stationary and time-varying parameters for a specific year of output shows that the global sensitivity results can differ. If time-varying parameters are treated as stationary in a variance based sensitivity analysis approach and thus their relative variance is also treated as stationary, the variance of the output is apportioned inconsistently with the actual parameter evolution. In particular, such an allocation is wrong if the parameters vary greatly in size over time.

Recommended Practice for Sensitivity analysis in dynamic material flow analysis

When it comes to sensitivity analysis in dynamic MFA, it boils down to the question of which sensitivity analysis approach is appropriate given the model structure and the output of interest. Considering the previous treatment of sensitivity analysis in dynamic MFA, this approach can expand the classification of sensitivity analysis in two important dimensions: On the one hand, time-delay effects of varying input parameters over the years when in use stocks are considered and, on the other hand, the observation of interaction effects if dependencies are given (multiplications are done) with values for which the probability density function attains the value zero with high probability (especially if a lot of other parameters depend on this value). Based on the findings of the sensitivity analysis of the archetypal dynamic material flow model and the review of the current state of the art of sensitivity analysis in dynamic MFA (see chapter 1.3.2), a recommended practice for sensitivity analysis in dynamic MFA is put forward. The corresponding, hierarchically ordered decision chart with the features of the observed model assumptions and the appropriate sensitivity analysis approach is shown in Figure 3.5. For systems which do not consider multiplications with parameters for which the probability density function attains zero, a variance based Fast Fourier Transformation algorithm (like EASI) can be used because it is sufficient to determine first order indices

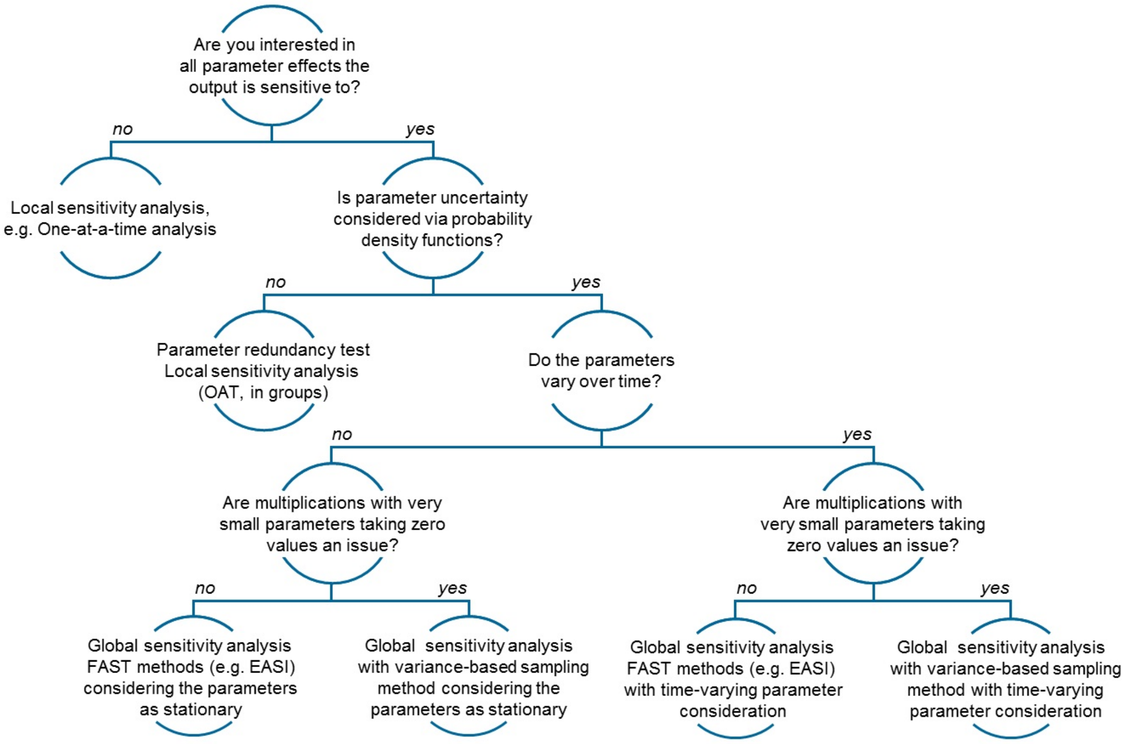


Figure 3.5: Decision scheme for selecting appropriate methods for sensitivity analysis in dynamic MFA [Source: II]

(main parameter effects), while cases which may have higher order effects can be solved with the variance based sampling method or with other methods proposed by Saltelli et al. (2009) which are more time efficient. Saltelli et al. 2009 proposes Jansen's estimator (Jansen 1999), radial sampling, and a quasi-random number method as the best estimators and as faster alternatives to the sample based approach for exploring higher order effects. The choice of method ultimately depends on the goal and scope of the analysis: Is it important to observe the whole system and every output of each time period or is it sufficient to explore the total effects on one output over one or two specific time periods? In the latter case, the variance based sampling method presented in this article is an appropriate choice.

3.3 Modeling structure evaluation

3.3.1 Results

The results of the comparison of the EOL wood flows and stocks, as well as for the substance flows are presented from a historical perspective together with cross-checks and future scenarios. Furthermore, the results are checked for the critical parameters.

Comparison of EOL wood flows and stocks

A comparison on EOL wood flow ranges (from demolition and renovation) between the leaching and delay approach together with cross-check data and its standard deviation (in the whiskers) is shown in Figure 3.6. The results are shown as mean values (black lines) together with the range of one standard deviation (i.e. 68% of the model results are contained in this range; indicated by grey area). The peak of the delay model is mainly caused by the dominating amount of roofs built before 1918 and ceilings and the high amount of floors from 1977-1997. Compared to these amounts of wood, the rest is of subordinate importance. Although the number of buildings in Vienna is rising in the future prognosis, the share of wood in buildings is remarkably lower from the end of the 20^{th} century on than it was in the beginning of the century. The peaks of the highest amounts of EOL wood are shifted for the two approaches. The reason are the high amounts of roofs built before 1918 leaving the stock 120 years later in the delay approach. In contrast to that, the main driver in the leaching approach is rather the size of the historical building stock, the roofs remain present for a longer period. The cross-checking value for waste wood and its standard deviation lie between the two model results, whereby the result of the mean value of the delay approach is very close

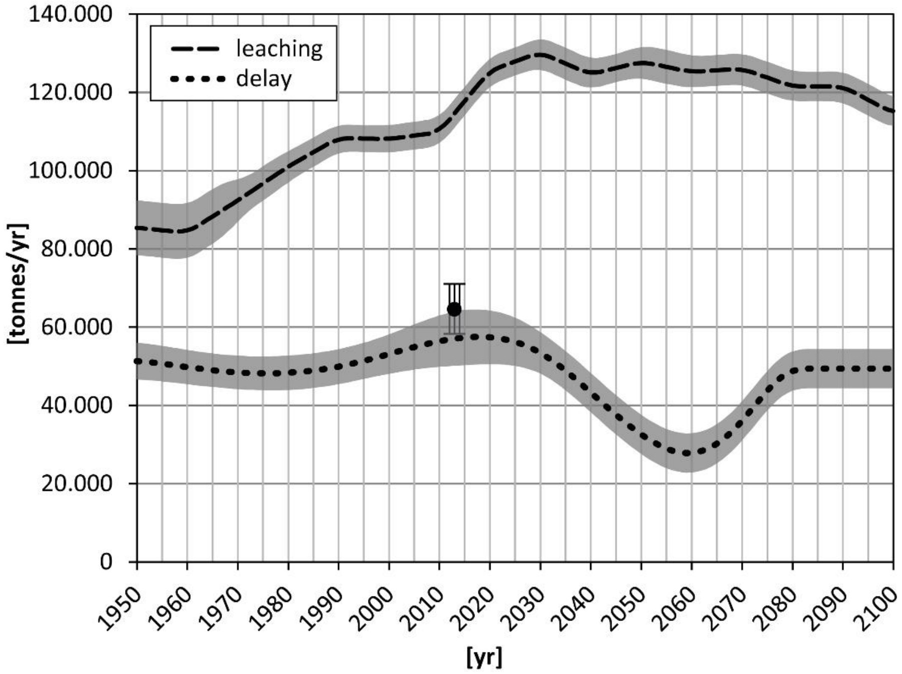


Figure 3.6: Flow of EOL wood from demolition and renovation activities [Source: III]

(and the range within the standard deviation) and the mean value result of the leaching approach far above this value. A comparison of the stock of the models reveals that not only the output flows are far higher in the leaching approach, but also the stock size is considerably higher. A major reason is that the technical lifetimes may be too short with regard to the initial stock. Very old wood components tend to be of better quality as they are made of solid wood in general, in contrast to present wood components, which mostly contain wood composites. Doubling these initial lifetimes in the delay approach leads to a stock size similar to the stock size in the leaching approach (see results in Article III).

Comparison of substance flows

In Figure 3.7, the comparison of lead in EOL wood flows is shown for the two approaches (mean values and ranges), in Figure 3.8, the comparison of chlorine, and the comparison of PAH in Figure 3.9. All substance flows show a similar behavior to the flow on the goods level in the leaching approach. This is due to the fact that the shares of the products over a period are aggregated. The contaminants lead, chlorine and PAH don‘t appear after 1996 or are replaced in wood products after 1996 respectively. Therefore, the flows are decreasing faster than the EOL wood flows. However, non-negligible values can still be found even after one century in the leaching approach. The highest amount of lead and chlorine can be found in wood from before 1918 (lead from windows and chlorine from ceilings), leading to high amounts at the beginning of the flow observations for both approaches. The share of this period is slightly shrinking in the leaching approach for both substance flows. There is almost no PAH in historical buildings from before 1918, which is reflected in the results of both approaches. The lead flow reaches another slight

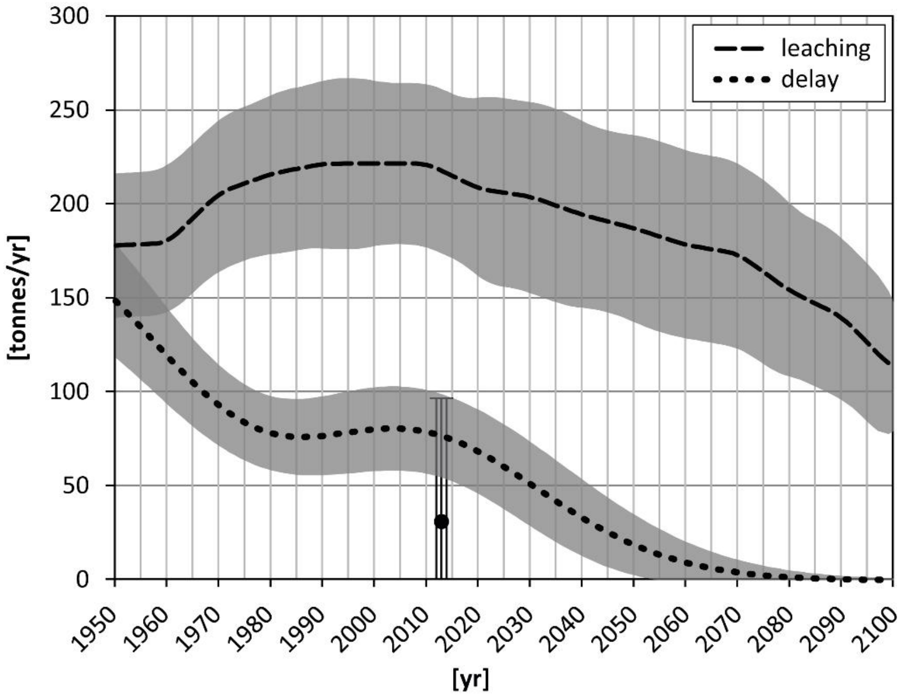


Figure 3.7: Lead flows in EOL wood [Source: III]

peak in the delay approach, resulting again from the high concentration of lead and the high share of windows input in the period 1946-1976. Windows have the highest amount of lead since lead was used for plastic coatings and color pigments. The comparison with the cross-checking data value shows that both models substantially overestimate the mean value (which may also be partly due to the high uncertainty of the estimate), but the range of the lead flow of the delay model lies within the range of the standard deviation. Ceilings and roofs from 1919-1945 have a slight impact on the chlorine flows observable in the delay approach. Chlorine was used as a hardener component in glue which was used for beams in wood. The cross-checking value of the average chlorine amount lies between both models, and is close to the result of the delay model. The growth of the PAH flow in the end of the 20st century in the leaching approach is caused by the rising amount of floors from 1919 on reaching their end of life. PAH from creosote was often used to stick parquet, but also as a preservative on windows. In the delay approach, the highest PAH flow value is mainly caused by the high amount

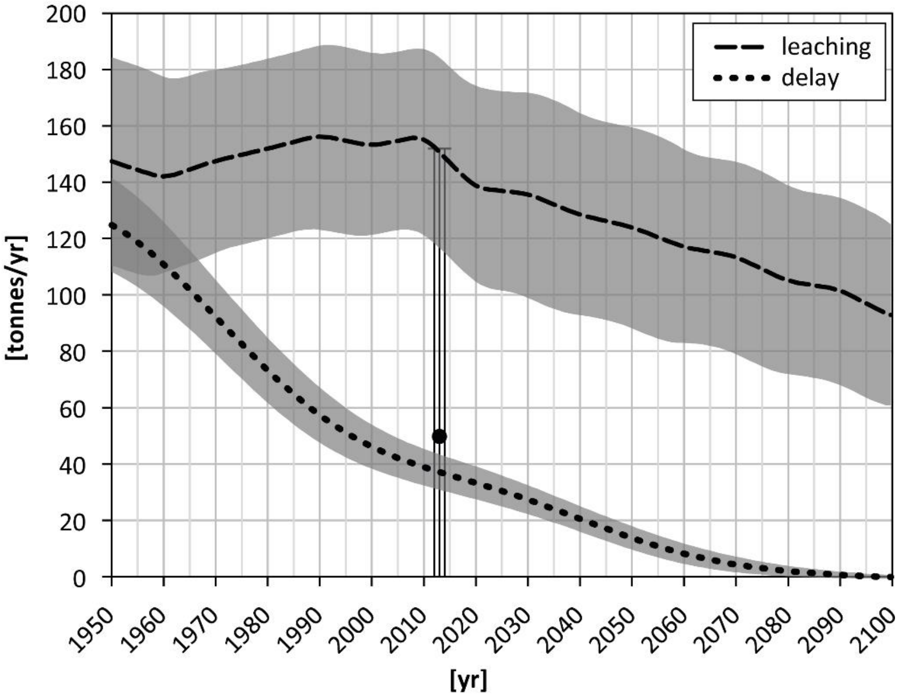


Figure 3.8: Chlorine flows in EOL wood [Source: III]

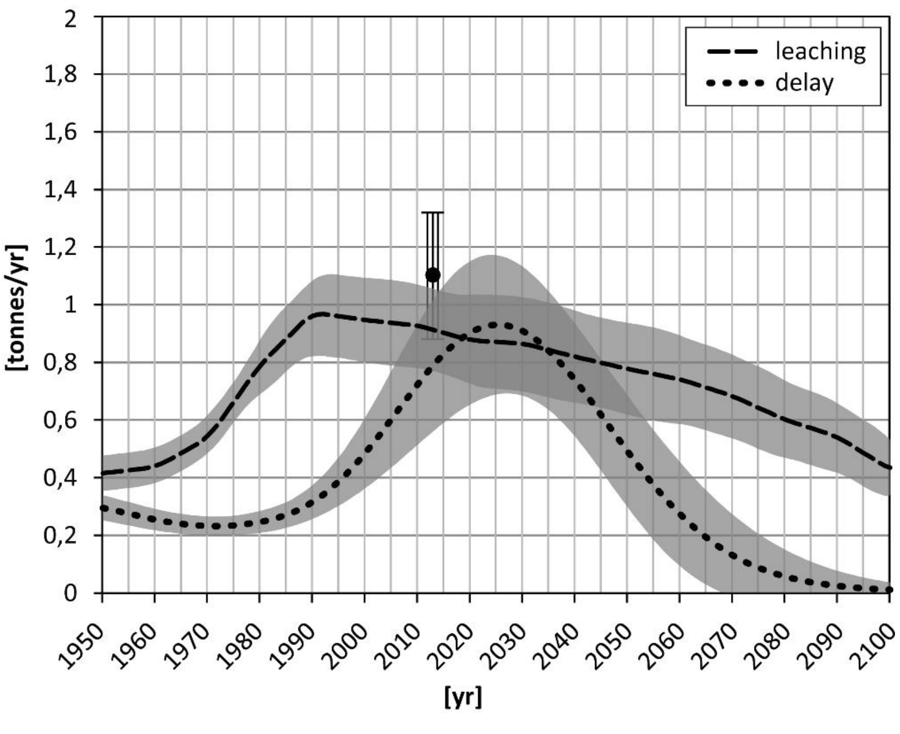


Figure 3.9: PAH flows in EOL wood [Source: III]

of floors from 1977-1997, and the high amount of floors and windows from 1945-1977. The amounts of PAH in other wood products are negligible. The cross-checking mean value for PAH is slightly underestimated by both approaches (both ranges lie within the standard deviation, though). One reason could be other PAH sources, e.g. roof tiles which partly adhere to the wood.

Results of sensitivity analysis

Local sensitivity analysis
Perturbations on the lifetimes in the delay approach and demolition and renovation rate in the leaching approach behave linearly with regard to the EOL output flows. Thus, in the delay approach, an increase in lifetimes goes hand in hand with an increase in the material stock as well as a decrease in output flows. Outputs from the leaching approach change directly proportional to changes in demolition and renovation rates. The effect of considering fewer buildings from before 1918 and therefore more of all other periods, is tested on the goods level. In both approaches, the reallocation of buildings into periods after 1918 leads to a drastic decrease of EOL wood flows. Historical effects of substance applications on current periods are tested on the example of PAH for the year 2010. PAH aggregations from the initial periods have the highest effect on the PAH output flow in the leaching approach, while the amount of PAH from 1977-1997 has the highest effect in the delay approach. This result is more reliable because for the leaching approach, the consideration that buildings from the initial stock are renovated with PAH-free wood is ignored, leading to an overestimation of PAH values from these periods.

Global sensitivity analysis
The first order effects are negligible for both modeling approaches, meaning that the uncertainty of the output is mostly determined by interactions of the parameters. Therefore, the uncertainty of the main effects of the bundled shares of wood constructions is analyzed. In the leaching approach, EOL wood flows are mainly sensitive towards the share of roofs and ceilings in buildings from before 1918. Because the wood content of modern buildings is relatively low and mainly constituted by floors, the share of floors becomes the most important model parameter during later model periods. The EOL wood flows in the delay approach have similar sensitivities. In a next step, the substance level of contaminants from EOL wood is considered. PAH flows are mainly sensitive to the floor parameters in both approaches from 1980 on, as floors are not only the main constructions in modern buildings but also have very high concentrations of

PAH. Chlorine flows are mainly sensitive to the share of ceilings in both approaches, as the concentration of chlorine in ceilings is tenfold higher as for all other wood constructions, and as the share of ceilings built before 1918 (the period with the highest wood content) is high. As for the lead flows, the concentration of lead in windows is tenfold higher than for every other wood construction, the share of windows is the main sensitive parameter for the lead flows in both approaches.

3.3.2 Discussion

Analysis of the EOL wood flows on goods and substance level

As the largest flow of EOL wood is related to roofs and ceilings from initial periods before 1918, and as in the future, the amounts of EOL wood will decrease because of the low share of wood in modern buildings, the peak of wood amounts which can be used as secondary resources is rather in current periods and won't play such an important role in the future. More pronounced downwards trends can be observed for the (banned) substance flows. However, the amounts of the contaminants still deplete slowly. Consequently, the contaminants are expected to still be present in low levels in EOL wood during the next 50 years.

Comparison of modeling approaches

EOL wood flows

A major drawback of the leaching approach, and main contributor to uncertainty in the results is that the demolition and renovation rate are always taken with regard to the whole aggregated stock to calculate the output flows, ignoring the age of the buildings, and leading to highly overestimated amounts of waste wood. However, this drawback is of little importance for the future estimations of the amount of EOL wood under the scenario assumption that the buildings in future periods will have the same wood content as nowadays (cf. results in van der Voet et al. 2002). In the delay approach, the input in the building period is unknown and an uncertain assumption. Together with the fact that technical lifetimes are not always representative for the demolition/renovation of buildings (particularly, for the initial stock of buildings), this approach is very uncertain from a fitting of model and data perspective under the given circumstances. However, with respect to EOL wood flows, the delay approach appears to result in more plausible estimates. The highest share of waste wood in Vienna originates from buildings before 1918 which will be renovated with the same amounts of wood and which will remain in stock. A shortcoming of the delay approach is that this is not accounted for, which leads to a potential underestimation of future EOL wood flows.

Substance flows
The problem of taking a leaching share of the aggregated stock as an output is propagated from the goods level to the substance level in the leaching approach. Therefore, for chlorine and lead flows, the mean values of the approach results in drastically higher estimates than the cross-checking mean values. From a future perspective, even more inconsistencies arise on the substance level. As lead, chlorine and PAH were forbidden in 1996, buildings from earlier periods will also be free of contaminants after renovations. This is ignored by the leaching approach, leading to overestimated amounts of contaminants until the end of the modeling period. The substance flows may be slightly underestimated by the delay approach, as the wood containing the substances often resides longer in stock than the technical lifetimes (cf. initial lifetimes of EOL wood flows). However, the cross-checking with data on substance flows in waste wood shows that (at present) the estimated amounts of substances lie within plausible ranges. From a future perspective, this approach is reasonable, as all amounts of contaminants appearing after 1996 are only delayed outputs from previous periods. After renovations where all wood constructions have been replaced, even old buildings will be free of these contaminants.

4 Conclusions and Outlook

Scientific contributions to uncertainty treatment in MFA

The systematic investigation of material flows and stock of anthropogenic systems through MFA allows a new view on the anthroposphere. MFA can link anthropogenic activities with resource consumption and environmental loadings, and is a powerful tool for policy decision support in the fields of resource efficiency, urban planning and environmental protection (Brunner and Rechberger, 2014). As the problems addressed by MFA gain in importance now and will become even more important in the future, a rigorous consideration of uncertainty in material flow models is needed. In this work, the major limitations of uncertainty treatment in MFA studies are analyzed and novel approaches to deal with these limitations are explored in three studies, differing in problem formulations, critical assumptions and objectives.

In the first study, a general possibilistic framework for data reconciliation is presented and applied to a case study on wood flows in Austria. Compared to existing approaches for data reconciliation under fuzzy constraints, the developed framework is generally applicable, as it does not require triangular or trapezoidal membership functions. It can handle any kind of membership functions which results from the data characterization step. Therefore, the presented approach leaves little space for arbitrariness and input manipulation, as the only input needed are the collected data points and an evaluation of the data quality, allowing for more transparent and consistent balancing of the data within the material flow model. Applying the developed framework to wood flows in Austria, weaknesses in the database and the setup of the model could be identified. The model results consist of the possible ranges and the consistency levels of each material flow. The latter quantify the degree of agreement between the input data and the mass balance constraints of the model. Based on the investigation of three data characterization alternatives, it was possible to show a trade-off between the confidence in the data (i.e. the more confidence, the narrower intervals) and the resulting flow consistency levels. Exploring this trade-off provides a possibility to analyze the relationship between data characterization and the quality of data reconciliation, because the confidence in the data is directly linked to their agreement in the balancing model. This provides a basis for assessing MFA results from the perspective of data reconciliation: Poor agreement in the model does not justify high confidence in the data and vice versa. As material flow modeling is an iterative procedure, the developed framework allows for optimizing uncertainty characterization with respect to the consistency of the material flow model.

The second study is of dynamic nature and deals with the identification of critical parameters through global sensitivity analysis and the question, which sensitivity approach is appropriate, given the model structure and output of interest. The analysis of the archetypal dynamic material flow model (which is a typical part of dynamic MFA studies; in particular, studies on metals) focused on two dimensions and showed that for classical dynamic model set ups, higher order effects do not contribute significantly to the sensitivity of the results. Furthermore, the study showed that EOL flows are sensitive with respect to variations in lifetimes during unstable periods of output whereas variations in sector split have the dominant effect on EOL flows during stable periods. Another important analysis step which is drawn from the study is that time-dependent variables need to be checked for delayed effects of previous periods by treating them as separate variables for each significant period of change. A reduction can be made by neglecting parameter values in periods, which are too far off the observed year of output (i.e. if the output in a specific year is of interest for the analysis). Based on the findings of the sensitivity analysis of the archetypal dynamic material flow model and the current state of the art of sensitivity analysis in dynamic MFA, a recommended practice for sensitivity analysis in dynamic MFA is put forward.

The third study deals with dynamic MFA studies of uncertain model structure, which are exemplarily investigated via the building stock, as buildings differ strongly in lifetimes. It is unclear if the main drivers are the technical lifetimes of buildings, or the business cycle of the building industry. This lack of information on the structure has a great impact on the amount of EOL flows leaving the building stock. A lifetime-based delay approach and an economy-based leaching approach are presented. It can be concluded that, for historical observations and their influence on current periods, the delay approach is a better choice than the leaching approach. Furthermore, the delay approach is also more representative on the substance level. These recommendations can be transferred to other dynamic analyses of building waste flows on a goods and a substance level under similar assumptions, particularly if forbidden contaminants are traced back, and their influence on future periods is of interest. Although the delay approach is based on a lot of assumptions, and the input of buildings has to be derived from incomplete data, the results are more reliable than those of the leaching approach, which is ignorant towards the diversity of the building stock (cf. van der Voet et al. 2002). The leaching approach assumes that all buildings in stock have the same likelihood to be demolished or renovated, as renovations and demolitions are always considered for the aggregated stock. However, buildings built 50 years ago are more likely to be demolished or renovated than buildings built 20 years ago with half of the wood content. Overall, the most critical parameters in both approaches are related to the wood content of buildings, which may differ extremely from one period to another. In order to get more realistic results using the leaching approach, the model would need to be extended so that the leaching part is not taken from the aggregated stock but is time-dependent, making such a study very resource and data intensive. However, this would be irrelevant in cases of a highly homogenous building stock. For studies which analyze EOL flows associated with buildings of very similar material intensity, the leaching approach is an adequate and easily applicable method, provided that reliable data on renovation and demolition activities (over time) are available.

The findings of these studies can be used both for guidance on how to conduct a modeling approach and how to analyze the uncertainties within this approach, but also as a framework on how to set up the consideration of uncertainties in different, already given MFA studies, as the case studies represent the typical critical core sections of MFA studies.

Outlook on future research agenda

This work serves as a contribution to the treatment of uncertainty in MFA. However, as we considered only reduced studies, some questions and extensions still remain on the agenda of future research.

1. How should stock dynamics and recycling loops be treated in the fuzzy set-based approach to data reconciliation?
   In future, the generalized framework should be applied to more complex (but still static) MFA systems considering these problems in order to validate its practicality.

2. Considering dynamic material flow models, they will gain in complexity in the future, due to the consideration of various material quality layers (e.g. Buchner et al. 2015) or the requirement of closed mass balances applied to the model (e.g. Pivnenko et al. 2016). How should sensitivity analysis be used in these upcoming model set-ups?
   Because higher order effects are expected to become more prominent in such models, the investigation of parameter interaction effects and parameter dependencies (e.g. Mara et al. 2015) should become a major field for extending the use of sensitivity analysis in dynamic MFA.

3. When it comes to the uncertainty of model structure of dynamic studies on the building stock, recommendations were given, preferring the delay approach for studies with differing wood contents, and the consideration of substance levels. How can this approach be improved to give a more realistic picture of the amounts of EOL flows?
   The delay approach should be adapted to consider the persistent share of historical buildings in the stock. This is especially important for MFA studies of European cities. The effect of the choice of lifetimes (such as the lifetimes of the historic stock) can also be adapted by modification of external parameters which extend the duration in stock by leaving the buildings in a depleted pool, such as the effect of the business cycle on building demolition and renovation in this study. However, the consideration was purely didactic, because of a lack of data to derive meaningful parameter value estimates for the share which depends on this parameter in the delay approach. Therefore, future studies should consider such effects based on historic data and economic models.

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Appendix

Article I:
A fuzzy set-based approach to data reconciliation in material flow modeling

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Applied Mathematical Modelling, 43 (2016)

Applied Mathematical Modelling 43 (2017) 464–480

Contents lists available at ScienceDirect

Applied Mathematical Modelling

journal homepage: www.elsevier.com/locate/apm

A fuzzy set-based approach to data reconciliation in material flow modeling

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ARTICLE INFO

Article history:
Received 16 July 2015
Revised 20 October 2016
Accepted 30 November 2016
Available online 5 December 2016

Keywords:
Epistemic uncertainty
Fuzzy sets
Material flow analysis (MFA)
Possibility theory
Uncertainty characterisation
Wood budget

ABSTRACT

Material flow analysis is used to quantify the material turnover of a defined system, relying on data about flows and stocks from different sources with varying quality. In this study, the belief that the available data are representative for the value of interest is expressed via fuzzy sets, specifying the possible range of values of the data. A possibilistic framework for data reconciliation in MFA was developed and applied to a case study on wood flows in Austria. The framework consists of a data characterisation and a reconciliation step. Membership functions are defined based on the collected data and data quality assessment. Possible ranges and consistency levels (quantifying the agreement between input data and balance constraints) are determined. The framework allows problematic data and model weaknesses to be identified and can be used to illustrate the trade-off between confidence in the data and the consistency levels of resulting material flows.

1. Introduction

Material flow analysis (MFA) is a tool to quantify the flows and stocks of materials in arbitrarily complex systems [1]. MFA has been widely applied to investigate resource and recycling systems, providing useful information regarding the patterns of resource use and emissions to the environment (e.g. Chen and Graedel [2], Müller et al. [3]). The material flow model consists of processes which are connected via flows [1]. The basic principle of MFA is the law of mass conservation. Therefore, the sum of inputs needs to be equal to both the sum of outputs and potential changes in stock for every process in the model (cf. Eq. (1)). Flows and changes in stock for each process are the unknown variables within the system which need to be balanced by linear equations of the form:

$$\sum_{i=1}^{n} f_{in_i} = \sum_{j=1}^{m} f_{out_j} + \Delta s, \tag{1}$$

where Δs is the stock change ($\Delta s < 0$ if the outflow exceeds the inflow) [4]. In order to balance the material flows and changes in stock in the system, data needs to be collected. These data typically originate from various sources with different data generation methods, quality standards and reporting schemes (cf. Laner et al. [5]). Thus, MFA is naturally confronted with uncertainty to the extent that the available data captures the true values of the variables (flows and changes in stock) of the system under investigation. Therefore, if the number of unknown variables (= no input data available) is smaller

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http://dx.doi.org/10.1016/j.apm.2016.11.020

than the number of balance equations, inconsistencies between input data may arise given the mass balance constraints of the model. In such cases of overdetermined systems, data reconciliation can be used to balance the model and to further gross error detection in order to evaluate the plausibility of model results [6]. Data reconciliation in MFA is traditionally performed by minimising the squares of measurement adjustments (using the least squares method) [7]. This approach is implemented in the widely used MFA software STAN, which is a ready-to-use tool for doing MFA while taking into account uncertainty [8], and in combination with gross error detection, it is a well established approach in process engineering for identifying and eliminating errors in flow data of mass and energy balance systems [9,10]. Taking into consideration the possibility that material flow data may not be normally distributed, recent work was done by Cencic and Frühwirth [11] based on Bayesian statistics to perform data reconciliation of data with more general probability distributions in linear material flow systems. However, as the choice of specific probability density functions cannot often be justified in situations of vague information, alternative representations of uncertain quantities of an epistemic nature in environmental assessment models using possibility and fuzzy set theory were put forward (e.g. Chevalier and Teno [12], Benetto et al. [13], Clavreul et al. [14], Holtmann et al. [15], Tan et al. [16]). Possibility theory is a way of reasoning in the presence of uncertainty by expressing non-precise information with the use of membership functions (instead of probability density functions) by means of uncertainty characterisation and quantification [17]. So far, in a MFA context, fuzzy reconciliation approaches have been compared to the standard least squares approach to quantify material flows of resource and recycling systems [4,6]. These existing applications build on linear membership functions (either triangular or trapezoidal) to characterise the given flow variables within the reconciliation approach. However, because given flows in MFA are often calculated by combining several data (e.g. amount of a commodity multiplied with the concentration of the material under investigation), the use of linear membership functions to describe flow variables represents a limitation for the translation of available information to the fuzzified flow variables (cf. Laner et al. [6]). Therefore, it is the goal of this work to develop a generalised approach to data reconciliation in a possibilistic framework based on fuzzy input data and fuzzy balance constraints. The approach is able to rigorously deal with multiple input data for a single flow as well as overdetermined equation systems of the material flow model and allows for arbitrary membership functions. The benefit of the generalised fuzzy reconciliation approach to improving the underlying material flow data and to evaluating the quality of the material balances is illustrated via a case study on wood flows in Austria.

The paper is organised as follows: Section 2 presents the proposed framework, which is the key part of the paper, together with its application and related work on fuzzy sets and data assessment. In Section 2.1, a brief overview of fuzzy set theory and its application to data reconciliation problems is provided. In Section 2.2, the case study on wood flows in Austria is introduced and the data quality assessment and uncertainty characterisation procedures are described. The developed reconciliation approach is presented after that in Section 2.3, consisting of an uncertainty characterisation and a balancing of model and data step. Two alternative approaches to uncertainty characterisation are presented for comparison in Section 2.4. Calculations and results are presented in Section 3. Section 4 discusses the developed reconciliation approach with respect to those sensitive characterisation steps and in the light of other reconciliation methods. In Section 5, conclusions on the use of the generalised framework for reconciling fuzzy data in MFA are provided and an outlook on future research is given.

2. Related work and proposed framework

2.1. Fuzzy set theory

Introduced by Zadeh in 1965, possibility theory was initially invented to provide a graded semantics to natural language statements [18]. However, the usage of this theory was extended to several domains dealing with imprecise data [17]. A fuzzy set is a generalised version of a classical set, where each value either belongs to the set or not. Every fuzzy set A^* is well-defined by its membership function:

$$\xi_{A^*} : M \to [0, 1], \tag{2}$$

mapping every value in M onto its "degree of belonging" to A^*. Unlike the indicator function of a classical set, for which the function value is either 0 or 1, the image of the membership function is the whole interval between 0 and 1. We focus on a special case of fuzzy sets with $M = \mathbb{R}$, called fuzzy numbers. It is always possible to apply the δ-cut method for a fuzzy number x^*, which means that, by definition, for every value $\delta \in (0, 1]$ the δ-cut:

$$C_\delta(x^*) := \{x \in \mathbb{R} : \xi(x) \geq \delta\} \neq \emptyset, \tag{3}$$

is a compact interval in $\mathbb{R}$. The interval

$$supp(x^*) := \{x \in \mathbb{R} : \xi(x) > 0\}, \tag{4}$$

is called the support and

$$cr(x^*) := \{x \in \mathbb{R} : \xi(x) = 1\}, \tag{5}$$

the core of the membership function. The support covers all possible values for a fuzzy number, whereas the core represents those values with complete membership. Every membership function of a fuzzy number is uniquely defined by its family of δ-cuts, which are nested intervals, and the degree of membership $\xi(x)$ for an arbitrary $x \in \mathbb{R}$ is given by the largest $\delta \in$ [0,1]

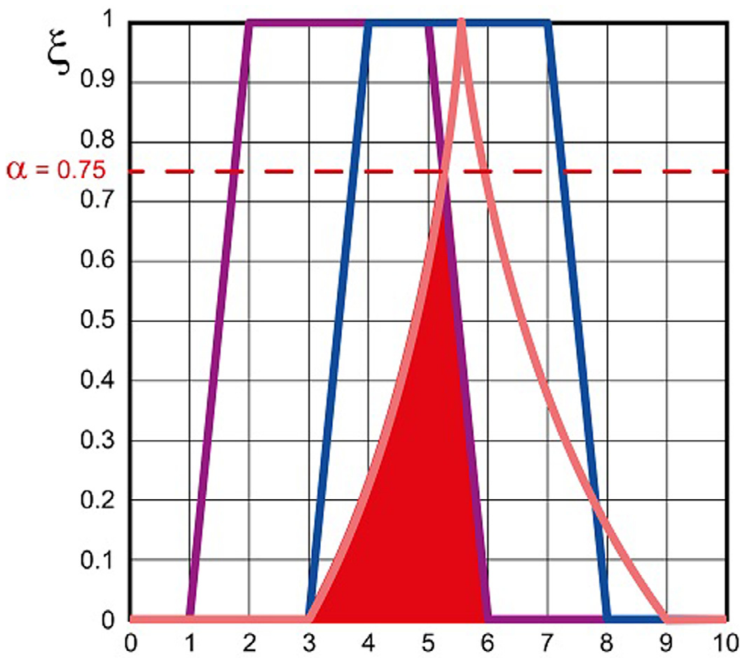

Fig. 1. The degree of consistency α is the maximum level of the intersection ξ^* of the membership functions ξ_1, ξ_2 and ξ_3. (For interpretation of the references to colour in this figure, the reader is referred to the web version of this article).

with $x \in C_\delta$. When dealing with computer programs, a sufficient number of δ-cuts is needed to describe a fuzzy number. The union of membership functions is defined as the maximum of them for each value on the x-axis, and the intersection as the minimum. The maximal value of the intersection of the membership functions $\xi_1, , \ldots, \xi_n : \mathbb{R} \to [0, 1]$,

$$\alpha = max_x\{min_x\{\xi_1(x), \ldots, \xi_n(x)\}\} \in [0, 1], \tag{6}$$

is known as the degree of consistency.

An illustrative example is given in Fig. 1. Three membership functions are considered, given by intervals of the form [a, b, c, d], where [a, d] denotes the support and [b,c] the core. $\xi_1 = [1, 2, 5, 6]$ and $\xi_2 = [3, 4, 7, 8]$ are trapezoidal and $\xi_3 = [3, 5.5, 9]$ has legs of a curved shape and its peak in 5.5 (b = c). The intersection of those three functions has a curved and a linear leg ($\xi^* = [3, 5.2, 6]$, highlighted in red). The peak is attained in 5.2. The degree of consistency of the intersection is 0.75 as this is the maximal function value ($\alpha = \xi^*_{max} = \xi^*(5.2)$). Operations on fuzzy numbers such as union and intersection, addition, multiplication and subtraction can be treated separately by operating on the intervals of each delta cut [19]. Fuzzification generalises a crisp (discrete) number and transforms it into a fuzzy (continuous) form by determining a range of possible variation for the support and a range of highly possible variation for the core. De-fuzzification transforms fuzzy numbers into crisp numbers. Fuzzification and de-fuzzification are used in interval-based reconciliation. The method for de-fuzzification is arbitrary and there exist several approaches, like using the centroid of the membership function as the de-fuzzified value. In this paper, the arithmetic mean of the core is used.

2.2. Case study on Austrian wood flows

Wood is a renewable resource with many different applications. Material uses of wood as construction materials, in furniture or in other products conserve the resource and therefore (potentially) enable another use of wood at the end of the product lifetime, either via energy recovery or material recycling. However, only vague information is available on the efficiency of wood processing in various industries and the management of waste wood flows. In addition, the variety of wood trade units (such as solid cubic meters [m^{3s}], cubic meters [m^3], metric tonnes [Mg], metric tonnes of dry mass [Mg dry matter], heating value [MJ], or pieces [pcs]) pose an additional challenge for balancing wood flows. Due to the challenges with respect to data availability and imprecise information, wood represents an ideal resource for testing the fuzzy reconciliation method. The focus of the case study is on a subsystem of the Austrian wood system for the year 2011. In order to validate the approach, we concentrate on five processes, namely the Sawing industry, the Boards industry, the Building timber industry and the Furniture industry as well as the Use-phase of wood products containing the in-use stock (see Fig. 2).

All other related processes, which are linked to the investigated system by flows, are defined to be outside of the system boundary and regarded as import and export flows of the system (= external flows). The flows within the system boundary are denoted as internal flows. There are no recycling loops considered in this subsystem. The major interest of the case study is in wood flows; historic stocks of wood are not investigated. Detailed information on the case study can be found

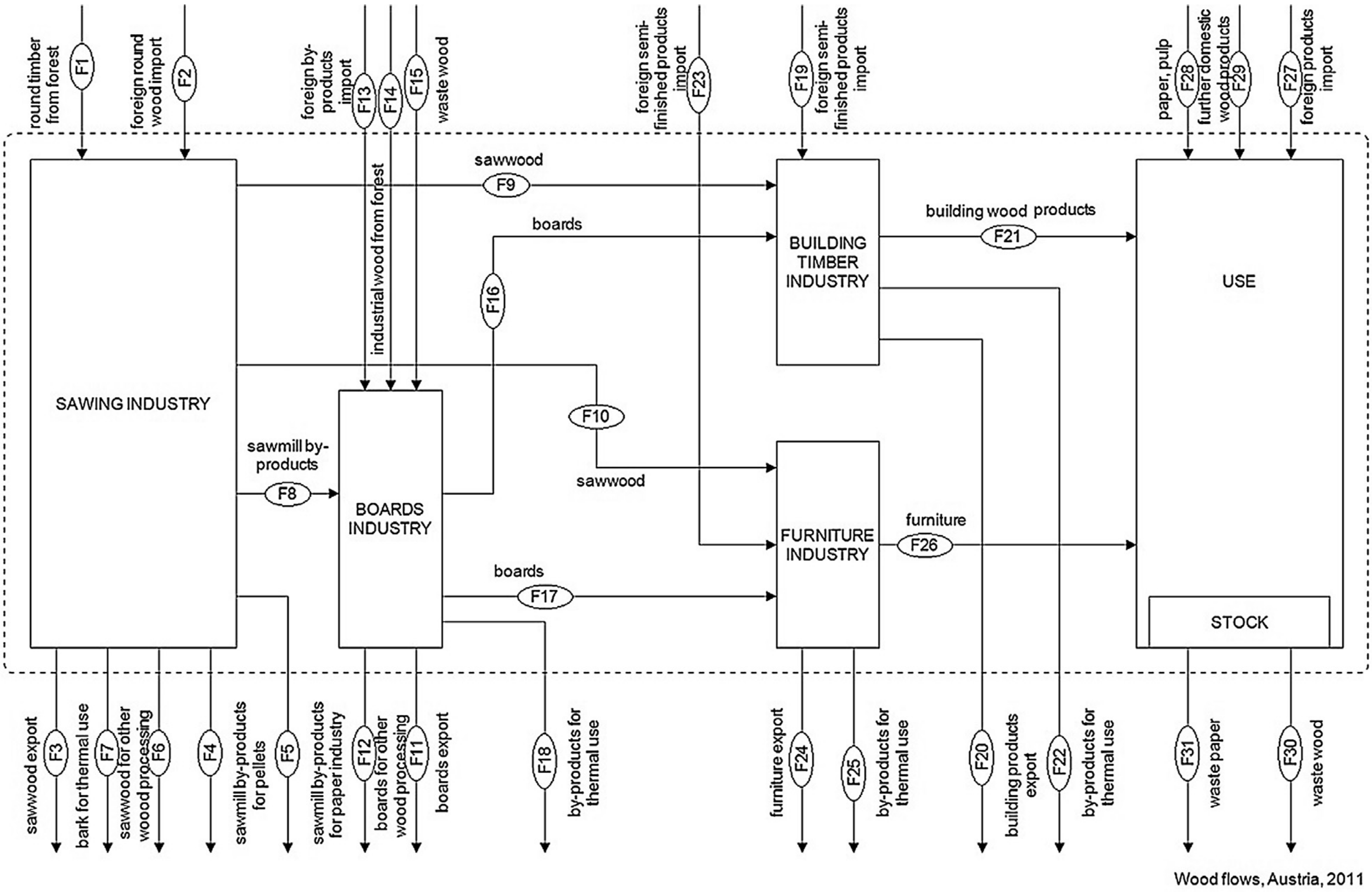

Fig. 2. Wood Flow model for Austria in 2011.

in the Supporting Information (SI) (SI-1). Assuming that there is no uncertainty attached to the model equations, the flow and stock change variables are forced to comply with the five mass balance constraints given by the processes considered in the model (cf. Fig. 2):

1. Sawing industry: $f_1 + f_2 = f_3 + f_4 + f_5 + f_6 + f_7 + f_8 + f_9 + f_{10}$
2. Boards industry: $f_8 + f_{13} + f_{14} + f_{15} = f_{11} + f_{12} + f_{16} + f_{17} + f_{18}$
3. Building timber industry: $f_9 + f_{16} + f_{19} = f_{20} + f_{21} + f_{22}$
4. Furniture industry: $f_{10} + f_{17} + f_{18} = f_{24} + f_{25} + f_{26}$
5. Use: $f_{21} + f_{26} + f_{27} + f_{28} + f_{29} = f_{30} + f_{31} + \Delta s$

Various data sources were used. Among others, these include data from Austrian national statistics [20], UN Comtrade import and export statistics [21], the national logging report [22] as well as data published by the industries, e.g. the Austrian paper industry [23]. Detailed information about the data sources can be found in the SI (SI-2 Tables 1–3). In most cases, one value is found to describe a certain flow (= uniquely defined flows); for some flows, 2 or 3 sources of information were available (= overdetermined flows). The quality of the data varies significantly. Some numbers are based on rough estimates, e.g. wood products, where the wood content is unclear. Other sources, such as the imports for the sawing industry, are precise and reliable. As the system needs to have the same unit for balancing in order to perform data reconciliation (to obey the mass conservation law), some unit conversions are required. In this work, we use tonnes of dry wood, which describes the wood content only and is therefore subject to mass conservation (i.e. fluctuations in water contents can be disregarded in the balancing). The collected data are shown in Tables 2–5. These data were used to describe the flows within the constructed system. The only variable remaining unknown is the stock change Δs in the use-phase. This means that only constraints (1)–(4) can be used for data reconciliation, because constraint 5 is needed to calculate Δs. Hence, the flows 27–31 are entirely determined by the input data membership functions. Δs is an unknown variable which is calculated through constraint (5).

2.2.1. Data quality assessment

The collection and aggregation of the data are essential parts of MFA. The quality of the data varies a lot and needs to be categorised. Four levels are assumed for the data quality assessment, taking reliability of the source as well as representativeness into consideration. Level 1 stands for relatively precise data based on official statistics and level 4 represents rough

Table 1
Classification of data.

Level	Source/reliability	Representativeness	Example	u_f
1	National statistics office/ independent institutions	National data	Data on imported wood from National cooperation plattform	1.09
1	Research studies	Numerous measurements of quantity of interest	Water content of waste paper from Statistics Austria	1.09
2	Statistics from interest groups or associations	National data	Data on imported semi-finished boards from the annual report of Austrian industries	1.20
2	Research studies	Estimated measurements or measurements not fully representative for the quantity of interest	Average conversion factor of all types of roundwood given by the Austrian energy agency (m^{3s} to tonnes)	1.20
3	Expert estimates	Data based on aggregation of expert estimates	Data on wood import in semi-fin. products aggregated by Austrian energy agency	1.44
3	Research studies	Measurements of limited representativeness	Average water content in waste wood based on water content of roundwood given by the Austrian energy agency	1.44
4	Rough estimates or educated guesses	Speculative estimates on aggregations based on scarce information	Estimated wood content of imported semi-fin. products for furniture based on trade statistics data	1.98

Source: Based on Laner et al. [6], adapted from Hedbrant and Sörme [24].

estimates. Apart from that, intermediate level values are also possible. The classification according to the levels is shown in Table 1 [6,24].

2.2.2. Characterisation of uncertainty

By means of those levels, the uncertainty factor u_f is computed for each collected data point according to a method by Hedbrant and Sörme [24] by assuming a continuous function. A comparison between linear and exponential uncertainty factor functions can be found in Laner et al. [6]. In this approach, an exponentially growing function:

$$u_f = 1 + ae^{bl}, \tag{7}$$

is assumed, whereby a, $b > 0$ are fitting parameters and l is the level. Parameter a controls the shift of the exponential curve on the y-axis and b can either stretch or compress the curve [24]. The uncertainty factors have a direct influence on the quantitative uncertainty of data. The value d is obtained by the formula (c.f. [24]):

$$\frac{(u_f - 1)}{2} = d, \tag{8}$$

which is later on used to define a range.

2.3. The reconciliation model

2.3.1. Approach for uncertainty characterisation in the model

The usage of an explicit function to derive uncertainty ranges guarantees for a consistent characterisation because it defines a transparent relationship between uncertainty scores and quantitative uncertainty estimates. Further information on the internal consistency of uncertainty characterisation can be found in Laner et al. [6]. However, the definition of the parameter values is subjective [25]. In this approach, $a = 0.04$ and $b = 0.8$ are chosen to fit the model in an appropriate way in order to end up with feasible solutions. The uncertainty range for data with level 1 is $d = 4.5\%$ of the original value, for level 2, $d = 9.9\%$, for level 3, $d = 22.0\%$, and level 4, $d = 49.1\%$. According to this range, the categorised data is fuzzified for each flow and stock change in the mass balance system by defining membership functions of either trapezoidal or triangular shape. Input data is divided into 3 groups: quantities, conversion factors for differing units, and commodity distributions to allocate percental shares of aggregated quantities to the flows and changes in stock. For simplification, we use the notification flows for both flows and changes in stock for the time being.

Table 2
Data on quantities used to establish the wood balance (sources: SI-2 Table 1).

f	Origin	Destination	Commodity	Dimension	Value in mio	Level
1	forest	sawing ind.	round wood	m^{3s}	11.797	1
2	import	sawing ind.	round wood	m^{3s}	5.360	1
3a	sawing ind.	export	sawwood	m^3	5.716	1
3b	sawing ind.	export	sawwood	m^3	5.591	1
4a	sawing ind.	pellet ind.	by-products	m^{3s}	1.793	2
4b	sawing ind.	pellet ind.	by-products	t fresh mass	0.900	1.5
4c	sawing ind.	pellet ind.	by-products	t dry matter	0.567	1.5
5	sawing ind.	paper ind.	by-products	m^{3s}	2.904	1
6	sawing ind.	other w. proc.	sawwood	m^3	3.934 (11%)[a]	1
7	sawind ind.	thermal use	bark, off-cuts	m^{3s}	3.251	2.5
8a	sawing ind.	boards ind.	by-products	m^{3s}	1.985	1.5
8b	sawing ind.	boards ind.	by-products	m^{3s}	2.000	1.5
9	sawing ind.	building ind.	sawwood	m^3	3.934 (78%)[a]	1
10	sawing ind.	furniture ind.	sawwood	m^3	3.934 (11%)[a]	1
11a	boards ind.	export	boards	m^3	2.600	2.5
11b	boards ind.	export	boards	m^3	2.400	2.5
12	boards	other w. proc.	boards	m^3	0.400 (9%)[a]	2
13a	import	boards	semi-fin. prod.	m^{3s}	1.017	1.5
13b	import	boards	semi-fin. prod.	m^{3s}	0.950	2
14a	ind. wood	boards ind.	ind. wood	m^{3s}	0.914	1.5
14b	ind. wood	boards ind.	ind. wood	m^{3s}	0.900	2
15	waste wood	boards ind.	waste wood	t fresh mass	0.280	2
16	boards ind.	building ind.	boards	m^3	0.400 (35%)[a]	2
17	boards ind.	furniture ind.	boards	m^3	0.400 (56%)[a]	2
18	boards ind.	thermal use	by-products	m^{3s}	0.374	2
19a	import	building ind.	semi-fin. prod.	m^{3s}	2.814 (78%)[a]	3
19b	import	building ind.	semi-fin. prod.	t dry matter	0.144	3
20	building ind.	export	products	t dry matter	0.854	3
21	building ind.	use	products	t dry matter	1.854	3.5
22	building ind.	thermal use	by-products	m^3	3.934 (9.72%)[a]	1
23a	import	furniture	semi-fin. prod.	m^{3s}	2.814 (11%)[a]	3
23b	import	furniture	semi-fin. prod.	t dry matter	0.030	4
24	furniture ind.	export	products	t dry matter	0.063	3.5
25	furniture ind.	thermal use	by-products	m^3	3.934 (2.16%)[a]	1
26	furniture ind.	use	products	m^3	0.667	2
27	import	use	products	t dry matter	3.278	3
28	paper ind.	use	products	t fresh mass	2.200	1
29	other w. proc.	use	products	t dry matter	0.100	4
30	use	waste wood	waste wood	t fresh mass	0.775	2.5
31	use	waste paper	waste paper	t fresh mass	1.434	1

[a] Data and the related levels refer to the original aggregated values; the actual flows are obtained by using the commodity distributions in brackets.

Table 3
Data on conversion factors to translate m^3 and m^{3s} into tonnes of dry matter (sources: SI-2 Table 2).

Flows	Commodity	Conversion factor	Unit	Level
f1, f2, f3, f6, f9, f10	roundwood	0.417	t/m^{3s}	2
f7	bark	0.393	t/m^{3s}	2
f7, f8, f13, f22, f25	off-cuts	0.417	t/m^{3s}	2
f5, f8, f13	sawdust	0.450	t/m^{3s}	2
f11, f12, f16, f17	boards	0.690	t/m^3	2.5
f14	industrial wood	0.417	t/m^{3s}	2
f11, f12, f16, f17	chipboard	0.500–0.650	t/m^3	2
f11, f12, f16, f17	mdf-board	0.800	t/m^3	2
f19, f23, f26	spruce wood	0.430	t/m^{3s}	3
f4	by-products in pellets	0.391	t/m^{3s}	3
f18	swarf	0.450	t/m^{3s}	3

Uniquely defined flows. Quantities are intuitively assigned trapezoidal membership functions. In general, if exactly one quantity is considered for a flow, the core of the membership function is defined by the interval $[x \pm d \cdot x]$ and the support by $[x \pm 2d \cdot x]$. Conversion factors and commodity distributions have triangular membership functions. The support is defined in the same way and the core is just the given data point x. In some cases, it makes more sense to define the membership functions in an asymmetrical way, e.g. for sawwood from the forest (see f1, Table 2) where excess lengths are considered. In order to convert a flow to the unit of the mass balance system or, respectively, to assign a flow with

Table 4
Data on conversion factors to translate tonnes of fresh mass (t fm) into tonnes of dry matter (t dm) (sources: SI-2 Table 2).

Flows	Commodity	Conversion factor	Water content (%)	Unit	Level
f4	by-products in pellets	0.920	8	t dm/t fm	2
f15, f30	waste wood	0.650	35	t dm/t fm	3
f28	paper	0.900	10	t dm/t fm	2
f31	waste paper	0.910	9	t dm/t fm	1

Table 5
Data on commodity distributions into different processes (sources: SI-2 Table 3).

Commodity	Origin	Destination	Fraction (%)	Level
boards	boards ind.	building ind.	35.00	3
		furniture ind.	56.00	
		other w. proc.	9.00	
sawwood	sawind ind. import	building ind.	78.00	3
	sawind ind. import	furniture	11.00	
	sawind ind.	other w. proc.	11.00	
by-products	furniture ind.	thermal use	2.16	4
	building ind.	thermal use	9.72	

Table 6
Comparison of α-levels for the processes.

Process	Base case	Reduced	Intersected
Sawing ind.	0.94	0.72	0.92
Boards ind.	1	0.81	1
Building ind.	0.97	0.74	0.77
Furniture ind.	1	0.99	1

the share of a common, aggregated quantity representing several flows, the quantity is transformed by multiplying its membership function by the function of the conversion factor (respectively, the one of the commodity distribution). The resulting function is usually neither trapezoidal nor triangular but rather of a curved shape.

Overdetermined flows. Overdetermined flows are treated by data fusion. To be precise, they are treated by a disjunctive approach to data fusion. This means that if one of the data sources (or its fuzzified version) regards a value as possible, it remains possible in data fusion [26]. Two scenarios are possible: a) data are homogeneous or b) data are given in different units or they do not relate to the same flow (i.e. the actual quantity of interest needs to be derived from aggregated data).

In the first scenario, the data points are merged into one trapezoidal membership function. For data which differ by less than 1 level (which is always the case in the present model), the arithmetic mean of data points is defined as the midpoint m of the core and support. Furthermore, the level is also defined as the arithmetic mean of the levels of the original data. The resulting uncertainty factor (u_f) is calculated out of the uncertainty function given in (7). In analogy to the uniquely defined flows, the core of the trapezoidal function is given by the interval $[m \pm d \cdot m]$ and the support by $[m \pm 2d \cdot m]$. If the data differ by more than 1 level, the focus is put on the more reliable data source by defining m as a weighted sum by taking the inverse of the uncertainty factors as weights (analogically, for the common uncertainty level). Again, in some cases, the membership function is slightly modified (but still trapezoidal) according to the context. If the data are not in the right unit, in the next step, multiplications are performed with the determined membership function so that it fits in the balance system.

In the second scenario, data needs to be harmonised before the final membership function can be identified for a flow. Heterogeneous data points are defined as distinct fuzzy intervals. Then, transformation is done by multiplying the fuzzy interval related to the original unit or quantity value by the membership function of either the corresponding conversion factor or commodity distribution or both. In the end, different membership functions of different shapes describe the same flow. By definition of the algorithm, they are merged together by summing up over the membership functions, normalising this sum (by dividing every value by the maximum), as this is a required assumption for the definition of fuzzy numbers and intervals, and taking the convex hull of this normalised sum. The resulting function can be a rather unusual, but convex shape (convexity is another required condition). Two alternative ways to deal with the fuzzification of input data are presented in Section 2.4.

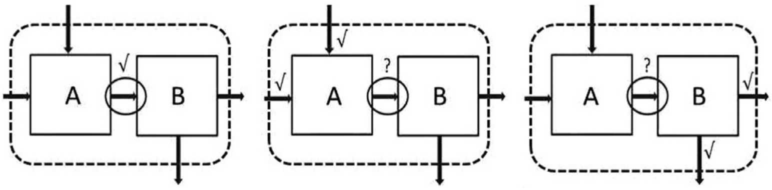

Fig. 3. This example shows the calculation of the membership functions belonging to an internal flow. On the left, the input data membership function is calculated. The other pictures show the functions resulting from the two balance constraints by assuming the internal flows to be unknown and by using fuzzy input intervals for the external flows.

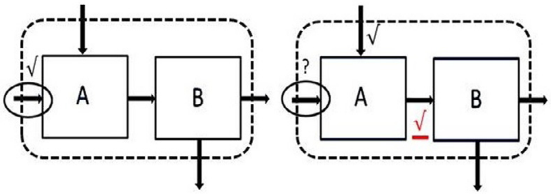

Fig. 4. In this example, the membership functions of an external flow are given. The left one is the input data membership function and the right one results out of the balance constraint. To calculate this constraint function, the internal flow resulting from step 1 is used while the remaining external flow functions used are based on input data.

2.3.2. Balancing of the model and data

In the end, every flow is represented by a single membership function based on the available input data. The membership functions of the input data have to comply with the mass balance constraints given in the model. The membership functions resulting from the balance constraints are obtained for each flow by assuming that the target flow is not determined and inserting all other input membership functions for the flows belonging to the same process into the balance constraint in order to calculate it. Thus, the reconciled fuzzy intervals are calculated via intersection of the membership function of the input data with the membership function(s) from the balance constraints. The reconciliation procedure consists of three major steps. An example of the case study's reconciliation steps is given in the SI (SI-3). The documentation of the reconciliation algorithm developed in Matlab can be found in the SI (SI-6).

- Step 1:
  In the first step, the membership functions resulting from the balance constraints are calculated for each internal flow (connecting processes within the system). Those functions are intersected with the membership function from the input data for each internal flow, and the degree of consistency α of the intersection of the three competing functions is calculated. An example of the three membership functions which are considered for an internal flow is given in Fig. 3. As the intersection function is only defined up to the maximal function value α, α is converted to a fuzzy interval by taking the interval on the level of α and keeping it fixed up to 1:

  $$C_\delta = C_{\delta^*}, \tag{9}$$

  $$\forall \delta \geq \delta^* : \delta^* := max_x\{min_x\{\xi_{input}(x), \xi_{constraint_i}(x), \xi_{constraint_j}(x)\}\},$$

  whereby i and j denote the processes which are connected by the flow. These extended functions are taken for further calculation in step 2. However, the basic intersection function and the level of α are also saved for step 3.
- Step 2:
  The fuzzy intervals for the internal flows are fixed. Then, the balance constraints are updated by inserting the internal flows as input variables. Now, the membership functions for all external flows are calculated using the updated balance constraints (one constraint per flow). Analogous to step 1, each of them is intersected with the membership function from the input data and the level of consistency is determined. Fig. 4 shows the membership functions of this step on the example already given in Fig. 3
- Step 3:
  The intersected functions within the system are normalised to 1 in order to obtain the fuzzy interval for each flow. The degree of consistency α is saved for each flow. As a result, the global consistency level is calculated, which is the minimal degree α of all flows under consideration.

Each process is described through one balance constraint. Thus, all flows which are only attached to one process (external flows) are linearly dependent. Therefore, the consistency levels are the same for those flows. The property does not hold for internal flows as they are described by two balance constraints, on the one hand, and calculated in advance, on the other. The relationships among the consistency levels of the flows are used to identify which ones are in poor agreement with the system. The global level of consistency is rather an indicator of the conflicts within the whole model or an indicator of model quality. A very low level of consistency could reveal wrong assumptions in the setup of the balance system. If the value is 0, there exists a flow with no intersection and, therefore, no solution at all. In the latter case, the system has to be updated.

2.4. Alternative approaches to uncertainty characterisation

Uncertainty estimates always remain subjective to some degree. Reconciled fuzzy ranges could be wrong even though flow data and balance constraints are in perfect agreement with high α-levels. It is assumed that the consistency of the model depends on the degree of uncertainty so that α-levels and, particularly, the global level of consistency can be adjusted by modifying the uncertainty factors attached to the data. Thus, being over-confident results in low consistency levels and small fuzzy ranges while being over-conservative results in high consistency levels at the cost of large ranges (c.f. Laner et al. [25]). In order to illustrate the trade-off between uncertainty ranges and consistencies, two alternative approaches to data characterisation are proposed. In the first approach, the uncertainty factors are reduced, which means more confidence in the data sources. In the second approach, the treatment of overdetermination of flows is modified by using a conjunctive approach to data fusion. Only values which are in the uncertainty range of any source are considered (c.f. Destercke [26]). The second approach also gives greater weight to the actual data sources and is useful in identifying problematic data efficiently (through high conflict in the input data).

2.4.1. Reduction of uncertainty ranges

In the first approach, the fitting parameter b of the uncertainty function in (7) is halved from $b = 0.8$ to $b = 0.4$. Thus, the uncertainty range d gets smaller, which results in narrower membership functions. This effect leads to higher conflict in the reconciliation step and, therefore, to lower degrees of consistency.

2.4.2. Intersection of input data

The second approach differs from the basic approach only for the flows with competing input data. In contrast to the disjunctive approach on data fusion, this modification makes every value impossible which is not part of all the membership functions defined for a flow. This means that instead of considering all possible values, only values which are not impossible are considered. First, competing data points are transformed to membership functions according to their uncertainty ranges. If the data points are homogeneous (i.e. in the same unit), the intersection of them is taken, α is saved and the function is normalised to 1 in order to get a membership function. The function is then multiplied by a conversion factor if it is not already in the system's unit. In the scenario of heterogeneous data points, the membership functions are first transformed, then intersected, and finally normalised. The final degree of consistency of a flow is defined as the product of the degree of consistency from the intersection of the input data (data characterisation) and the degree of consistency from the reconciliation process. This is done because the result should reflect both impacts, conflict in the input data and conflict in the reconciliation step. The basic and the reduced ranges approach don't reflect the conflict in overdetermined input data for a flow. The definition of the final degree of consistency as a product is tenable if it is assumed that in the basic and reduced ranges approach, the degree of consistency of the data characterisation step is 1. As the membership functions of the overdetermined flows become narrower, there is more conflict in the reconciliation, resulting in lower levels of consistency. Besides, because the consistency levels for the overdetermined flows are 1 at the maximum in the intersection step (in the case of perfect agreement), the levels are considerably lower than those defined in the initial approach (= base case). Two examples of the treatment of overdetermined data for the approaches presented are given in Figs. 5 and 6.

3. Calculation and results

The reconciliation algorithm is applied to determine the flows of the Austrian wood flow system. An interpretation of the results of the reconciled wood flow model in the base case can be found in the SI (SI-4). The results are compared among the three approaches to characterise the input data taking the reconciled ranges and the achieved consistency levels into consideration. De-fuzzified values are used to derive statements about the wood flows. The fuzzy intervals are transformed to crisp values by taking the arithmetic mean of the core interval as the de-fuzzified value.

3.1. Comparison of approaches on uncertainty characterisation

The results of the alternative data characterisation approaches are depicted in Figs. 8 and 9. The core is listed in the upper part and the support in the lower part of each flow trapezoid. The de-fuzzified value indicates the thickness of the flows. The colour scale denotes the level of consistency for each flow. The scale ranges from purple, indicating very low consistency, to dark blue, which stands for perfect agreement. Grey denotes the flows which are not affected by the reconciliation process. These belong to the use-process only as the process has one degree of freedom, because the change of stock is not given by input data, i.e. a calculation result. The colour scale highlights that the α-levels consistently decline for the reduced ranges case compared to the base case, as all flows noticeably change the colour to either light blue from navy (e.g. the boards industry) or to purple from turquoise (e.g. the sawing industry). The same consistency rule with less discrepancy on the colour scale holds for the intersected data approach in comparison to the base case with the exception of the intersected flows, which have the lowest consistency levels (e.g. flow 19 or flow 4, shown in purple).

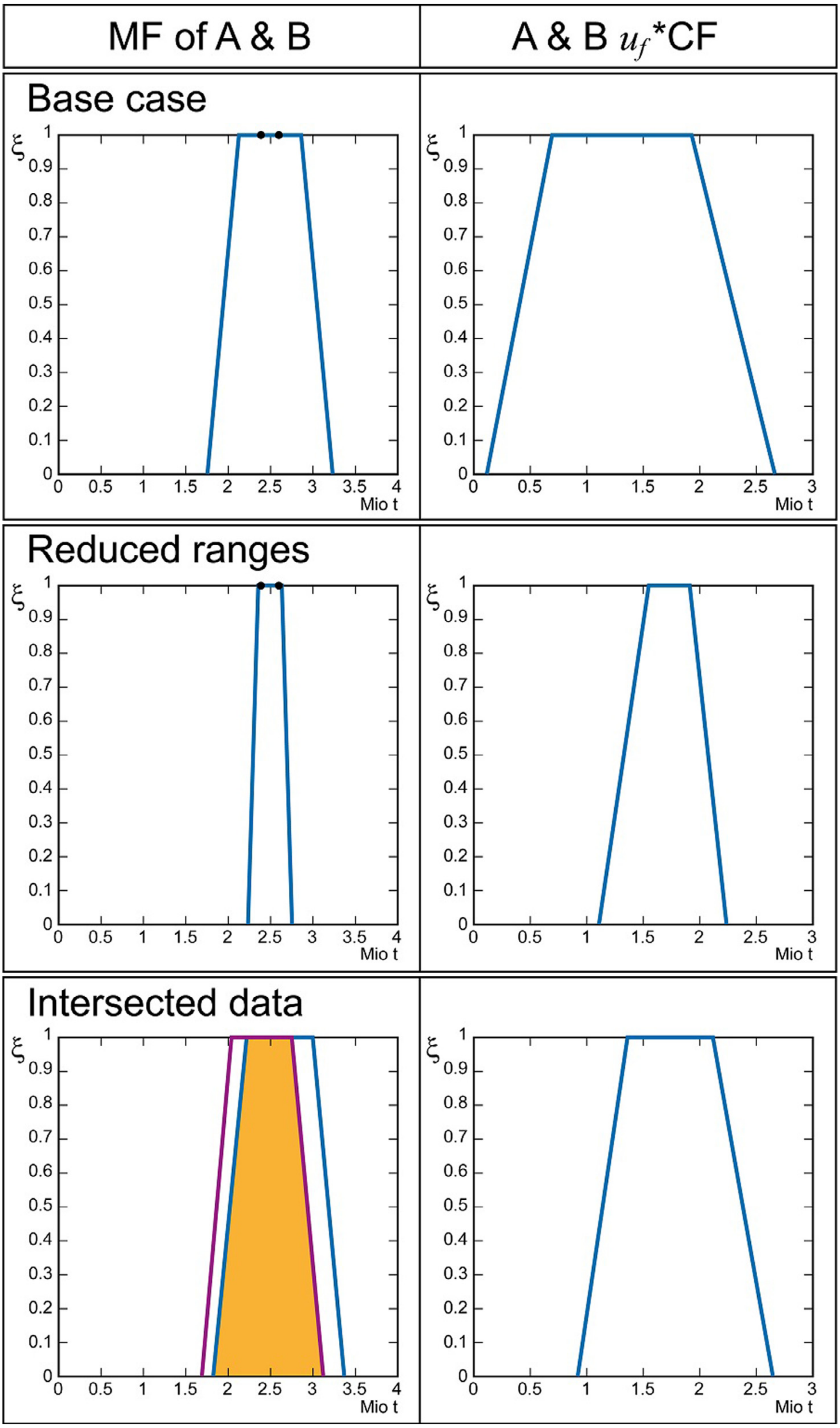

Fig. 5. This example shows flow 11 of the Austrian wood flow model for the different approaches on data characterisation data for homogeneous data points. The given data points A and B are in the same unit. They are first merged together and then converted in the system's unit.

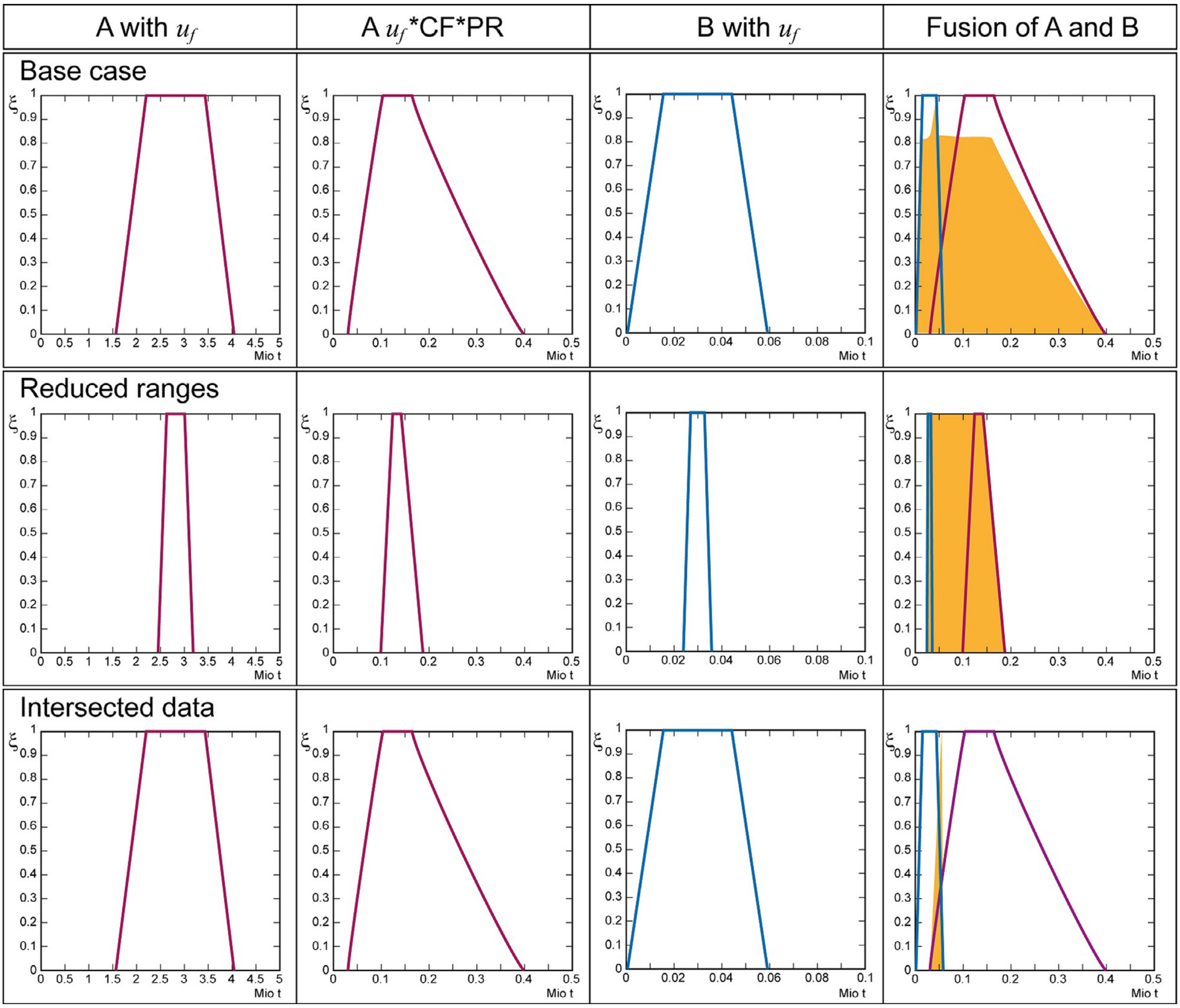

Fig. 6. This example shows flow 23 where two heterogeneous data points are given. In order to assign them to the flow, A needs to be converted into the system's unit and transformed in the right proportion first. Then, they can be merged together.

3.1.1. Comparison of consistency levels

As indicated by different colours in the figures, all flows related to only one process are linearly dependent and share the same level of consistency. The degrees of consistency of the processes are given in Table 7. The α-levels for the processes are quite high for the base case, the global level of consistency, which is the level of the sawing industry process (0.94) indicating very good agreement between the fuzzy ranges. Reducing the ranges causes a reduction in the consistency levels of the sawing industry process of approximately 24%, and a further 19% for the building timber industry process. Those are the processes with the lowest consistency levels. However, comparing the intersected data approach to the base case, there is only a significant change for the building timber industry, with a 20% lower consistency level. This is due to the fact that the changes in the reconciliation step are caused only by the narrower fuzzy intervals of the overdetermined data. The α-levels for internal and overdetermined flows are given in Table 8.

The intersected data approach has the lowest α-levels for the overdetermined flows with heterogeneous data points (flow 4, 19 and 23). The relative change in the internal flow consistency levels to the base case is less than 26% in any of the alternative approaches. Thus, reducing the ranges of the input data by halving the fitting parameter b in the exponent of the uncertainty factor function reduces the consistency of the flows on average to around 18%. Although the relative change in the global level of consistency for the intersected data approach is almost 93%, most of the levels for the flows remain the same and thus, the average change is only 9%. This confirms the trade-off between uncertainty characterisation and consistency levels because the levels decrease when more trust is given to the input data.

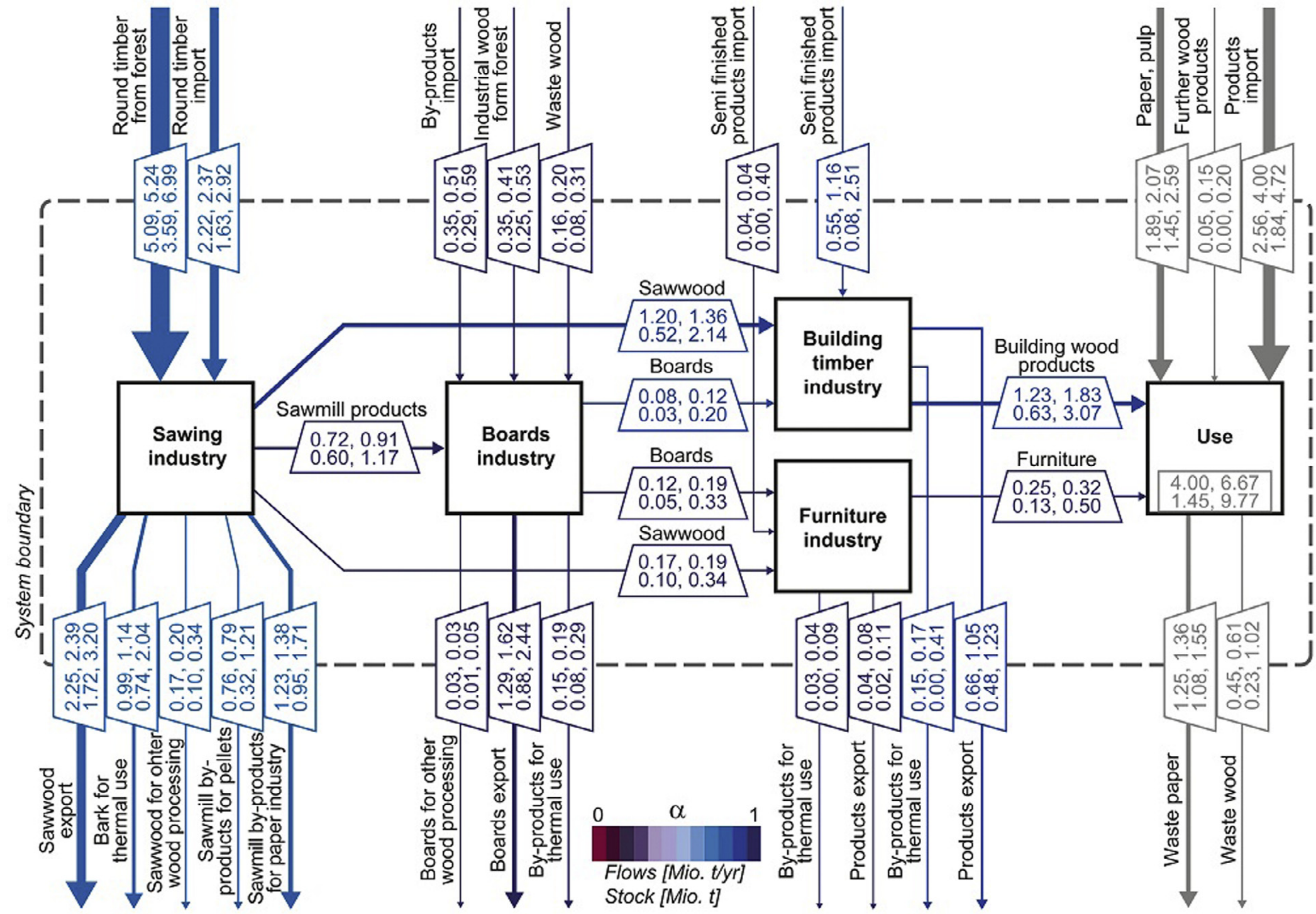

Fig. 7. Reconciled wood flow model.

Table 7
α-levels for internal & for overdetermined flows.

Flow	Base case	Reduced	Intersected
3	0.94	0.72	0.92
4	0.94	0.72	0.26
8	1	0.79	1
9	0.97	0.72	0.77
10	1	0.79	1
11	1	0.81	1
13	1	0.81	1
14	1	0.81	1
16	0.97	0.82	0.77
17	1	0.99	1
19	0.97	0.74	0.07
23	1	0.99	0.36

3.1.2. Comparison of reconciled fuzzy ranges

Considering Figs. 7–9, it can also be observed that each approach gives slightly different results for the reconciled fuzzy ranges. In contrast to all other flows, the fuzzy ranges for f19 are greatly different. They vary from [0.08,0.55,1.16,2.51] in the base case to [0.37,1.13,1.14,1.55] in the reduced ranges approach, and [0.16,0.20,0.21,0.21] for the intersected data approach. The changes in reconciliation results of the de-fuzzified flow values for the base case as well as for the two alternative approaches in comparison to the original data points are given in Table 9. The original data points are transformed by crisp multiplications with the data points given for conversion factors and commodity distributions. If a flow is overdetermined, the arithmetic mean of the data points is used as the original value. The flows f4, f8, f10 and f19 share the particular feature in that the direction of the changes in the mass flow in comparison to the input data is different for the three different approaches. While the reconciled value of f4 increases for the base case and the reduced ranges, it declines for the intersected data approach. The same trend holds for f19, which is also a heterogeneously overdetermined flow. Conversely, flows f8 and f10, which are both internal flows and therefore restricted through two balance constraints, decrease for the base

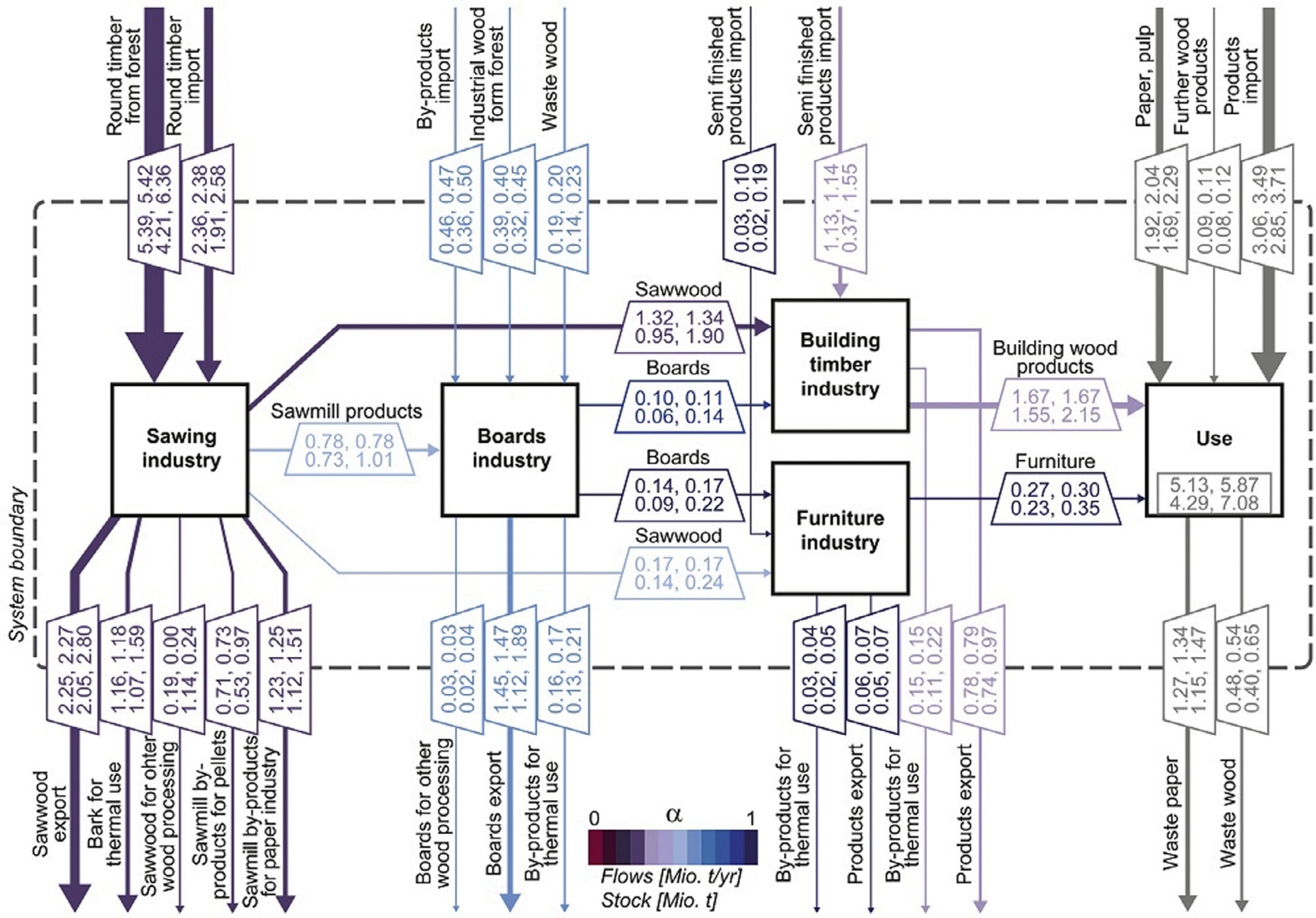

Fig. 8. Reduced ranges. (For interpretation of the references to colour in this figure, the reader is referred to the web version of this article).

case and the reduced ranges (apart from f10, which doesn't change in the base case) and increase for the intersected data approach. The diverse effect on f4 and f19 is caused by the uncertainty characterisation for overdetermined, heterogeneous flows. The fused data points lead to enlarged fuzzy input intervals in the base case and reduced ranges approach, which leaves a margin for the balance constraints. Thus, the balance constraints have a higher impact on those two approaches, causing increasing values in both approaches. In contrast to that, the constricted narrow fuzzy input ranges for the f4 and f19 have a higher impact than the constraints for the intersected data approach, leading to decreasing values (c.f. Table 9). The internal flows f8 and f10 are attached to the sawing industry process and therefore depend on f4. According to the balance constraint for this process, an increase in the value of f4 leads to an increase in the values of f8 and f10, and vice versa. This follows the effects shown in Table 9. The fact that the changes in the internal flow f9, affected by both f4 (sawing industry) and f19 (building timber industry), do not differ in sign is because the fuzzy ranges of the input and the balance constraints are far broader than those of f8 or f10. The effect of the narrow ranges of both f4 and f19 in the intersected data approach is strong enough to have a positive reconciliation effect on f9. However, the broad ranges of f4 and f19 for the base case and reduced ranges approach allow a broad range for the fuzzy solution of f9 so that their influence is negligible.

3.1.3. Detection of weaknesses

The foreign import of semi-finished building industry products f19 has the lowest global α-level in the intersected data approach, with 0.07. Moreover, this flow is also the one with the largest relative changes in the reconciled fuzzy ranges when comparing the different approaches (59.3% in the base case, 109.3% for the reduced ranges approach and -63% in the intersected data approach). This is caused by high conflict in the input data for f19. The values of the transformed data points f19a and f19b are so far off each other that at least one of them must be substantially flawed. It is difficult to ascertain which one because the uncertainty factors of both data points are relatively high. In order to get a better understanding of the magnitude of this flow, the wood flow model is tested without these data points for the base case by treating f19 as a free variable. The resulting de-fuzzified value is 1.52 Mio t, which is closer to the input data of f19a $= 0.944$ Mio t than to f19b $= 0.44$ Mio t. Therefore, f19b is ignored in the next step and the system for the base case is again reconciled by considering only f19a as an input date for this flow. The reconciled, de-fuzzified value is then 0.94 Mio t, i.e. f19 remains almost unchanged after the reconciliation step. Although the global level of consistency is the same as the initial result, the α-level of the building industry can be raised to 1 so that all processes except for the sawing industry (unchanged with $\alpha =$

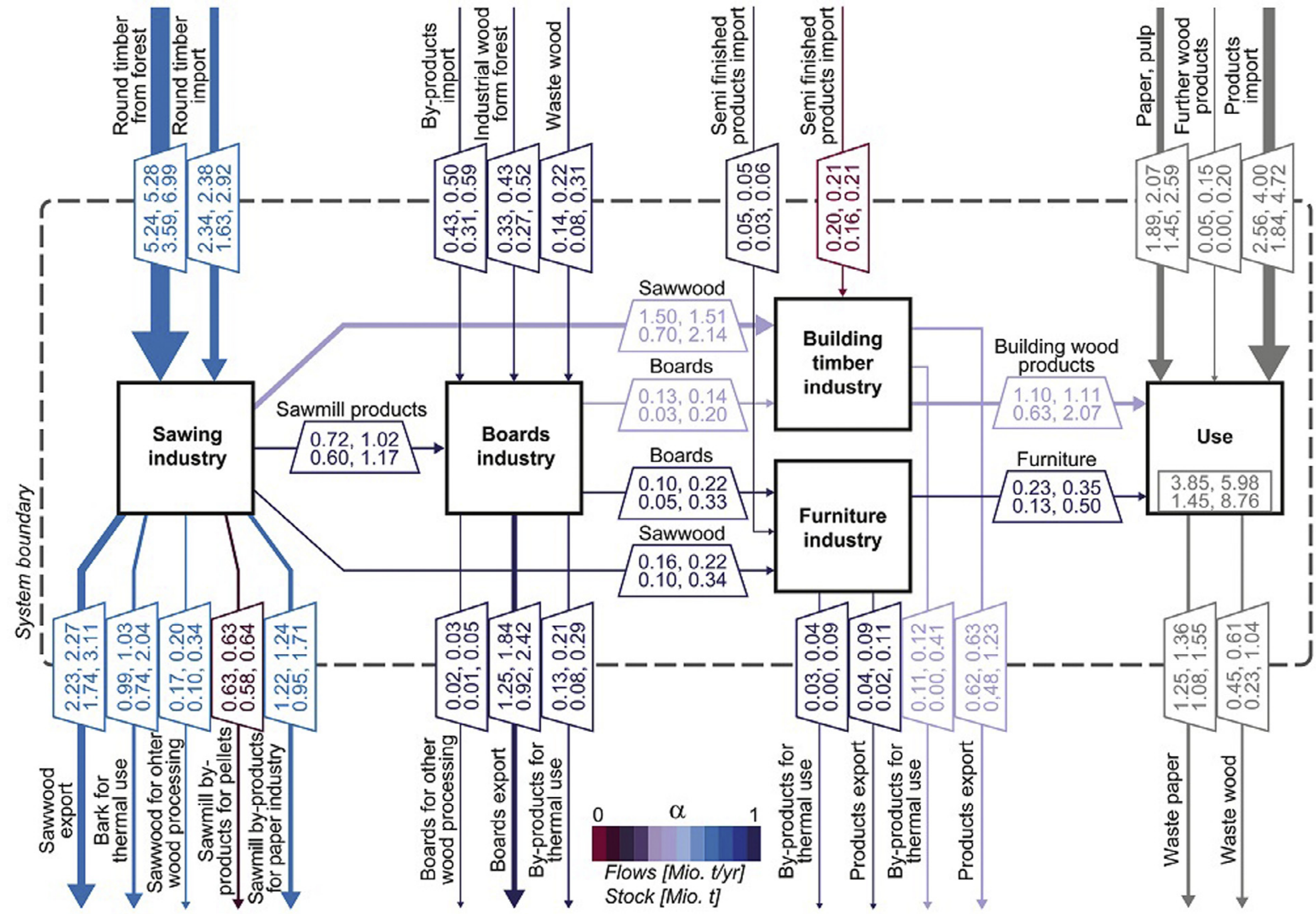

Fig. 9. Intersected data. (For interpretation of the references to colour in this figure, the reader is referred to the web version of this article).

0.94) have perfect consistency with $\alpha = 1$. Both of the de-fuzzified values for f19 (without considering the data for f19 and by considering f19a only) would be covered by the reconciled fuzzy intervals for f19 in the base case and reduced ranges approach, but not in the intersected data approach (where 0.21 Mio t is the maximal possible value).

4. Discussion

4.1. Reconciliation algorithm

The fact that the output of the developed approach contains not only the reconciled flows and their resulting uncertainty but also information about their consistency within the model is the main added value of the developed approach in contrast to other reconciliation methods. A recommendation for consistency level benchmarks is given in Table 9. This indicates the agreement of the data for a flow within the model and is also a benchmark for the global degree of consistency. α-levels above 0.9 stand for excellent agreement. It is assumed that α-levels beyond 0.5 are acceptable while all values below indicate poor agreement. In the latter case, the data (or the model) is in need of an update.

The existing Linear programming method for reconciliation under fuzzy constraints is only applicable to membership functions of triangular or trapezoidal shape. However, as most of the flows result from multiplications with conversion factors or commodity distributions, the resulting membership functions are rather of a curved shape. Thus, using a linear program, the results are inaccurate as the intersection points may be shifted. This can lead to big deviations of membership functions through error propagation (cf. Laner et al. [6]). The generalisation to common membership functions is a main innovation of the developed approach. The required number of δ-cuts (approximating a continuous function) in order to get reliable results depends on the magnitude of the data values considered. The number of observed digits ν_1 plus significant decimal digits ν_2 determines the amount of δ-cuts $N = 10^{\nu_1+\nu_2-1}$. As single-figured numbers with two digits are considered for the Austrian wood flows, the membership functions are split into 100 δ-cuts and the x-axis is observed up to the 3rd decimal place (and rounded afterwards), so that errors lie within a $10^{-3} \times 10^{-2}$-square unit. Thus, precision up to the second digit can be assumed.

Table 8
Comparison of the changes in the reconciled, de-fuzzified flow values relative to the crisp input data (transformations done without fuzzification) and of the change relative to the total contribution to changes (the sum of all absolute changes) due to reconciliation.

Flow	Input	Base case		Reduced		Intersected	
	Crisp	Total contribution to changes (%)	Relative change (%)	Total contribution to changes (%)	Relative change (%)	Total contribution to changes (%)	Relative change (%)
f1	4.91	15.4	5.3	20.3	10	11.7	7.1
f2	2.24	3	2.2	5.4	5.8	4	5.4
f3	2.36	−2.4	−1.7	−4.1	−4.2	−3.7	−4.7
f4	0.7	4.7	11.4	0.8	2.9	−2.3	−10
f5	1.31	−0.6	−0.8	−2.9	−5.3	−2.3	−5.3
f6	0.18	0	0	−3.7	−50	0	0
f7	1.32	−14.8	−18.9	−6.2	−11.4	−10.3	−23.5
f8	0.86	−2.4	−4.7	−3.3	−9.3	0.3	1.2
f9	1.28	0	0	2.1	3.9	7.3	17.2
f10	0.18	0	0	−0.4	−5.6	0.3	5.6
f11	1.73	−16	−15.6	−11.2	−15.6	−6.3	−11
f12	0.03	0	0	0	0	0	0
f13	0.43	0	0	1.7	9.3	1	7
f14	0.38	0	0	0.8	5.3	0	0
f15	0.18	0	0	0.4	5.6	0	0
f16	0.1	0	0	0.4	10	1	30
f17	0.15	0.6	6.7	0	0	0.3	6.7
f18	0.17	0	0	−0.4	−5.9	0	0
f19	0.54	18.9	59.3	24.5	109.3	−11.7	−63
f20	0.85	0	0	−2.5	−7.1	−7.3	−25.9
f21	1.85	−18.9	−17.3	−7.5	−9.7	−24.7	−40
f22	0.16	0	0	−0.4	−6.3	−1.3	−25
f23	0.08	−2.4	−50	−0.8	−25	−1	−37.5
f24	0.06	0	0	0	0	0	0
f25	0.04	0	0	0	0	0	0
f26	0.29	0	0	0	0	0	0

Table 9
Recommendation for consistency level benchmarks

α	Agreement
>0.9	Excellent
>0.7	Good
>0.5	Fair
0.5–0	Poor

4.2. Effect of uncertainty characterisation

How can a system with no or poor agreement be updated to get a feasible solution or a solution with higher consistencies? The problem may be due to uncertainty ranges which are defined too narrowly. If a very low level of global consistency cannot be increased by an appropriate enlargement of uncertainty ranges, the first step should be to check input data for potentially erroneous data sources related to the problematic flows or processes, respectively. Full reliability of the model is assumed since the constraints are fixed and not uncertain. A poor global α is also an indicator of problems arising with respect to the consistency of the balance system's assumptions. If it is not possible to improve the input data in order to rise global α in an appropriate way, the balance system (i.e. the model) should be critically reconsidered with respect to correctness and completeness. This iterative way of improving data and model is typical for the procedure of doing an MFA (cf. Brunner and Rechberger [1], Laner et al. [5]).

Considering the Austrian wood flows, the three different approaches on uncertainty characterisation result in widely varying consistency levels. The trade-off between uncertainty ranges and consistency levels provides a better understanding of the way the data should be characterised. The highly conservative characterisation of uncertainty in the base case leads to large ranges and excellent consistencies, which is not really representative if the data quality is considered. Besides, the scope of the flow ranges leaves a lot of leeway in the reconciliation process. In the present case study on wood flows, the preferred uncertainty characterisation approach is the reduced ranges approach. While all fuzzy ranges become more precise, the loss in consistency is modest compared to the base case. According to the global degree of consistency, the system can still be referred to as good and therefore reliable as well as coherent, but not optimal, which also confirms the impression from model construction and data collection. Larger, more complicated balance systems with similar data quality assessments should be treated by using the base case. The intersected data approach points out the weaknesses within the wood flow system. The global degree of consistency is almost zero, which means that the wood flow model is untenable and in need of change. This is true for flow 19 as can be seen in Section 3.2.3. However, no update of the system would lead to errors in the reconciliation results of the intersected data approach. This can be seen on the instance of f19, where the de-fuzzified values, which result from ignoring f19 and also from ignoring the obviously wrong data point f19b, are outside of the range of the reconciled fuzzy interval of the intersected data approach. As relatively many overdetermined flows are considered for these (and especially also larger) wood flow systems, this approach requires a lot of revision and adaption to obtain acceptable consistencies according to Table 9. This is not worthwhile in this simple, five-process case study because the gain in information through the reconciled values of this approach is not so high. A comparison of the base case and reduced ranges approach with the updated systems (e.g. for f19) lead to no significant changes in the fuzzy ranges of the flows through reconciliation.

4.3. Comparison to existing fuzzy-based approaches

The reconciliation approach developed in this work was analysed by comparing it to the lexmin approach with fuzzy linear programming used by Dubois et al. [4]. Furthermore, the reconciliation approach to the case study on Austrian wood flows was compared to the standard least squares approach using the software STAN [8], as was done by Dubois et al. [4] in order to validate the leximin approach (see Fig. 1 and Table 4 of SI-5 in the SI). The application to the Australian copper system, taken over from van Beers, van Berkel and Graedel [27] allows the usage of the linear program as each of the flows is uniformly defined by a triangular membership function. In this reconciliation approach, all flows belonging to the process with the lowest degree of consistency are fixed to the singletons attained in the core of the membership functions. Then, the reconciliation step is updated with the next higher α-level. The step is repeated until all flows are fixed to singletons. Except for some differences in the system's assumptions, it was possible to reproduce the results of the leximin approach with the algorithm presented because for linear problems of such symmetrical shape, there exists only one optimal solution. However, in a more general case, more weight would be given to the flows with the lowest consistencies by using the leximin approach. It should be reiterated that linear programming is only applicable to simple case studies with triangular or trapezoidal membership functions and leads to imprecise results if multiplication is considered and a generalised approach is needed. The multiplication of trapezoidal functions results in a distribution with curved legs instead of straight ones, leading to error propagation in the reconciliation step when linearised instead of curved fuzzy sets are intersected (see SI of Laner et al. [6]). As membership functions need to be cut into slices in order to perform reconciliation in the general case, it is very time consuming to always fix the flow intervals with the lowest consistencies and iterate the procedure until all of them are fixed. The method presented in this paper offers a more practical approach since it consists of only two reconciliation steps. As the internal flows are attached to all processes and, therefore, their reconciliation affects all other flows in the next step, it is natural to reconcile them in the first step.

5. Conclusions

In this study, a general possibilistic framework for data reconciliation in MFA was presented and applied to a case study on wood flows in Austria. The framework consists of a data characterisation step and a reconciliation step. Uncertain input data are expressed via functions indicating the degree of membership of values within possible intervals. Compared to existing approaches for data reconciliation under fuzzy constraints, the developed framework is generally applicable as it does not require triangular or trapezoidal membership functions. It can handle any kind of membership function which results from the data characterisation step. Therefore, the approach presented leaves little space for arbitrariness and input manipulation, as the only input needed are the collected data points and an evaluation of the data quality, allowing for more transparent and consistent balancing of the data within the material flow model. By applying the developed framework to wood flows in Austria, weaknesses in the database and the setup of the model could be identified (e.g. the data basis concerning semi-finished wood product imports (flow 19) was found to be problematic). The model results consist of the possible ranges and the consistency levels of each material flow. The latter quantify the degree of agreement between the input data and the mass balance constraints of the model. Based on the investigation of three data characterisation alternatives, it was possible to show a trade-off between the confidence in the data (i.e. the more confidence, the narrower the intervals) and the resulting flow consistency levels. Exploring this trade-off provides a means to analyse the relationship between data characterisation and the quality of data reconciliation because the confidence in the data is directly linked to their agreement in the balancing model. This provides a basis for assessing MFA results from the perspective of data reconciliation: Poor agreement in the model does not justify high confidence in the data and vice versa. As material flow modeling is an iterative procedure, the framework developed allows for optimising uncertainty characterisation with respect to the consistency of the material flow model.

In the future, the generalised framework should be applied to more complicated MFA systems to validate its practicality for material flow models, including recycling loops and stock dynamics.

Acknowledgements

We would like to thank Oliver Cencic for providing useful comments on a previous version of this article.

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Supporting Information

A fuzzy set-based approach to data reconciliation in material flow modeling

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The Supporting Information provides background information to the case study on Austrian wood flows which was used to test the reconciliation method. Besides, an useful example for the reconciliation steps based on the case study is provided in order to get a better understanding of the balancing of model and data. In the end, the results of the reconciliation on the case study are compared to the results obtained by data reconciliation with a least squares approach.

Contents

1 SI-1:Explanation of the wood flow model

The following explanation serves for a better understanding of the case study on wood flows in Austria:
Raw wood, which is processed in the sawing industry, is either imported from abroad or taken from Austrian forests. Sawwood is then exported or sold, among other wood processing industries, to the furniture and building industry. Another important material, dealing with a competitive market, is the vast amount of incurred sawmill by-products. It is sold to the boards industry, as well as to the paper and pellet industry. Boards are either sold to the building timber, furniture and other industries or exported. Aside from by-products from the sawing industry, board production relies on imports of by-products, industrial wood, and waste wood. Customers of the boards industry are the building and the furniture industry, the production residues are incinerated. Within the domestic sawwood and boards, there are also imported semi-finished products used in the building and in the furniture industry. Both industries sell products domestically and abroad. Furthermore, for both industries incurring by-products from the production process are used thermally. The use-process includes all wood products which are either domestically manufactured or imported in the year 2011. The historic stock represents in-use wood products in Austria (not considered in this study). Waste wood and paper are the products leaving the system.

2 SI-2: Data sources for the Austrian wood flow model

The following Tables show the data sources for the flow quantities, conversion factors and commodity distributions which were used in the Austrian wood flows case study. If two sources are given for a flow, the first is the one which was found and the second one was given as a reference by the first source. The flows f6,f9,f10 and f22,f25 in Table SI-1 denote the same aggregated quantity. This quantity is partitioned with the commodity distributions for sawwood (f6,f9,f10) and for by-products (f22,f25) given in Table SI-3. The flows f12,f16 and f17 denote also the same aggregated quantity, partitioned with the commodity distribution for boards (Table SI-3).

Table 1: Quantities

Flow	Source
f1	Nemesthoty, Austrian Energy Agency [8], HEM
f2	Nemesthoty, Austrian Energy Agency [8], FHP [5]
f3a	Nemesthoty, Austrian Energy Agency [8], FHP [5]
f3b	Wood Industry Report [16], Statisitics Austria [12]
4a	Nemesthoty, Austrian Energy Agency [8], FHP [5]
4b	ProPellets Austria [9]
4c	Statisitics Austria [11]
5	Nemesthoty, Austrian Energy Agency [8], Paper Industry Austria [14]
6	Nemesthoty, Austrian Energy Agency [8], FHP [5]
7	Nemesthoty, Austrian Energy Agency [8], FHP [5]
8a	Nemesthoty, Austrian Energy Agency [8], FHP [5]
8b	Wood Industry Report [16]
9	Nemesthoty, Austrian Energy Agency [8], FHP [5]
10	Nemesthoty, Austrian Energy Agency [8], FHP [5]
11a	Schwarzbauer, Institute for Marketing & Innovation,BOKU [10]
11b	Schwarzbauer, Institute for Marketing & Innovation, BOKU [10]
12	Schwarzbauer, Institute for Marketing & Innovation, BOKU [10]
13a	Nemesthoty, Austrian Energy Agency [8], FHP [5]
13b	Wood Industry Report [16]
14a	Nemesthoty, Austrian Energy Agency [8], FHP [5]
14b	Paper Industry Austria [14]
15	Windsperger, Institute for Industrial Ecology, Austria [15]
16	Schwarzbauer, Institute for Marketing & Innovation, BOKU [10]
17	Schwarzbauer, Institute for Marketing & Innovation, BOKU [10]
18	Nemesthoty, Austrian Energy Agency [8], FHP [5]
19a	Nemesthoty, Austrian Energy Agency [8], FHP [5]
19b	UN Comtrade [13]
20	UN Comtrade [13]
21	Statisitics Austria, [11]
22	Nemesthoty, Austrian Energy Agency [8], FHP [5]
23a	Nemesthoty, Austrian Energy Agency [8], FHP [5]
23b	UN Comtrade [13]
24	UN Comtrade [13]
25	Nemesthoty, Austrian Energy Agency [8], FHP [5]
26	Windsperger, Institute for Industrial Ecology, Austria [15]
27	Paper Industry Austria [14]
28	Paper Industry Austria [14]
29	Statisitics Austria [11]
30	Windsperger, Institute for Industrial Ecology, Austria [15]
31	Paper Industry Austria [14]

Table 2: Conversion factors

Commodity	Source
roundwood	Nemesthoty, Austrian Energy Agency [8], FHP [5]
bark	Nemesthoty, Austrian Energy Agency [8], FHP [5]
off-cuts	Nemesthoty, Austrian Energy Agency [8], FHP [5]
sawdust	Nemesthoty, Austrian Energy Agency [8], FHP [5]
boards	Egger, Austrian Boards Company [4]
industrial wood	Nemesthoty, Austrian Energy Agency [8], FHP [5]
chipboard	Windsperger, Institute for Industrial Ecology, Austria [15]
MDF-board	Windsperger, Institute for Industrial Ecology, Austria [15]
spruce wood	Windsperger, Institute for Industrial Ecology, Austria [15]
by-products in pellets	ProPellets Austria [9]
swarf	Nemesthoty, Austrian Energy Agency [8], FHP [5]
by-products in pellets	Nemesthoty, Austrian Energy Agency [8], FHP [5]
waste wood	Nemesthoty, Austrian Energy Agency [8], FHP [5]
paper	Paper Industry Austria [14]
waste paper	Kalt, Austrian Energy Agency [7], Statistics Austria [12]

Table 3: commodity distributions

Commodity	Source
boards	Brandstätter, Austrian Society for Wood Research [1],
sawwood	Windsperger, Institute for Industrial Ecology, Austria [15]
by-products	Brandstätter, Austrian Society for Wood Research [1],

3 SI-3:Example on balancing of model and data

The following example on 8 and f11 on from the case study on Austrian wood flows is presented in order to explain the reconciliation steps in the balancing of model and data. The internal flows are reconciled in the first step of the balancing of model and data. Thus, f8 is calculated in a first step out of the intersection of the input data membership function and the balance constraints membership functions. The overdetermined, homogeneous input data membership function is calculated according to the presented scenario on uncertainty characterisation (c.f. Figure 2 for f11 of the manuscript). The other two membership functions result out of the balance constraints of the sawing industry process with the input flows for f1-f7 and f9,f10 and the boards industry process with the input flows f11-f18 (see Equation 1 and 2 from the case study in the manuscript). The intersection of the three membership functions is calculated on the analogy to the example given in 2.1 in the manuscript (cf. Figure 1 in the manuscript).
As the external flows are calculated in the second reconciliation step, f11 is calculated hereafter. This calculation of the input membership function for f11 is given in Figure 5 of the manuscript. This function is intersected with the membership function of the balance constraint from the boards industry process. This means, that f8 and f12-f18 are used to calculate f11, whereby the input membership function are used for f12-f18 and the result of the reconciliation in the first step for f8.
Both flows have an consistency level of 1 after the first two steps. Therefore, their normalisation in the third step ends up in the same membership functions.

4 SI-4:Results of the reconciled wood flow model in the base case

The following results show the interpretation of the reconciled model in the case study. The reconciled fuzzy intervals for the Austrian wood balance resulting from the model in the initial approach (−base case) are shown in Figure 7. Considering the de-fuzzfied values, the results indicate that 5.17 Mio tonnes of round timber from domestic forests are used in the sawing industry in 2011. More than 30% of the total amount of round timber that goes into the sawing industry is imported from abroad. The largest fraction of output of the sawing industry is exported sawwood (almost 30%) to other countries, followed by an enormous amount of sawmill by-products going into the paper industry (16.5%) and sawwood used for the building industry (about 16%). Almost 84% of the produced boards are exported, only a small fraction goes to the national industries. 46% of wood products are imported to Austria. The paper industry has the highest domestic production (and almost 28% of the total production from inland and abroad), followed by the building timber industry (making up 21% of the total production). Concerning the data quality, there exist relatively precise data sources for the sawing industry process. The data on the boards industry process are also relatively tenable. On the other hand, there are scarce reliable data available for the building and furniture industry. The unreliable data make it difficult to quantify wood flows to the use-phase.

5 SI-5: Comparison to the reconciliation results with STAN

The results of the fuzzy-set based approach on the Austrian wood flow model are compared to a standard least squares approach using the software STAN [2]. The STAN reconciliation results are given in Figure 1. The arithmetic mean value of the flow data (multiplicated with the arithmetic mean value of the conversion factor if conversion is needed) is used as the mean value of the normal distribution of the flows. The standard deviation is assumed to be 10% of this mean in each case like in the comparison of the leximin approach with fuzzy linear programming to the STAN approach in Dubois et al. 2014 [3]. A comparison of the STAN results to the results obtained by the fuzzy-set approach is given in Table 4. The highest relative changes are observed for f19 and f23, the flows for which the alternative approaches have the highest relative changes and low alpha-levels, too (see Table 7 and Table 8 in the manuscript). The detection of the weaknesses of this flows in the balancing would remain unexplored using the least squares approach, as their reconciled values (f19−0.54 and f23−0.08) are almost the same as the crisp input values (which are f19=0.54 and f23=0.08, see Table 8 in the manuscript).

Figure 1: The reconciled Austrian wood flows calculated with STAN

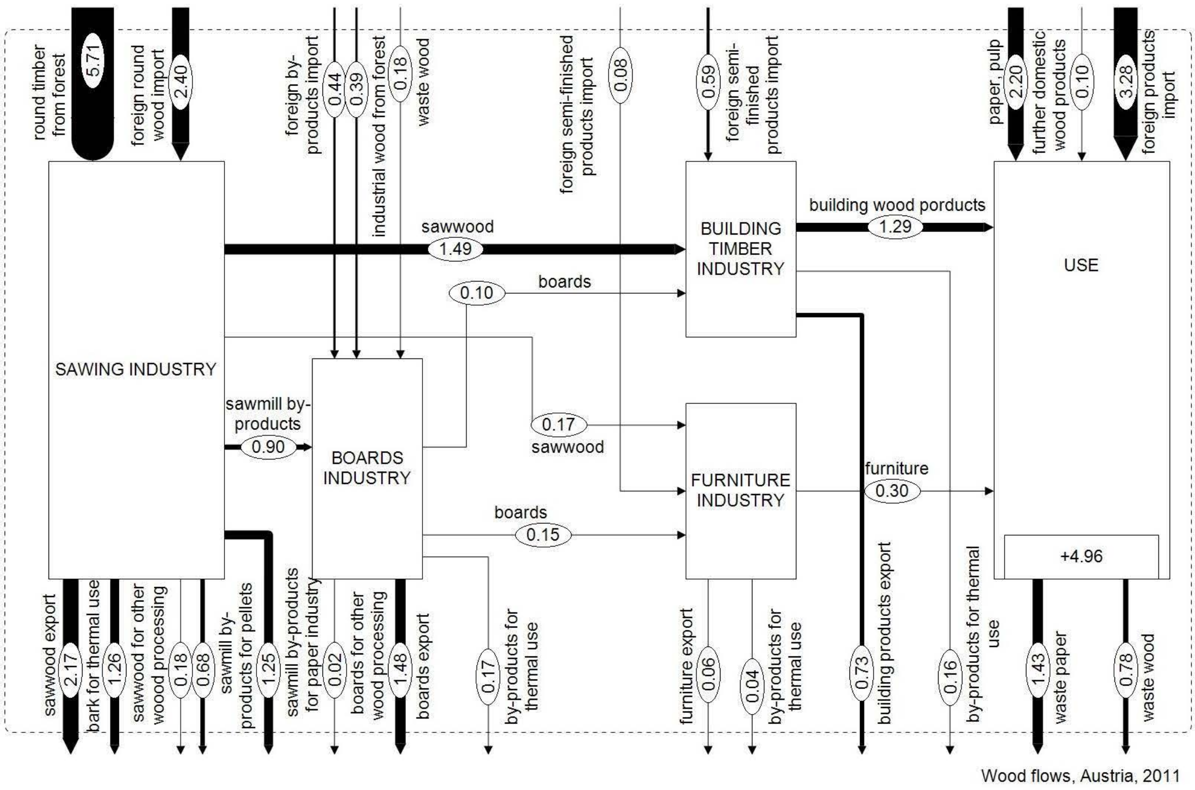

Table 4: Comparison of the results on the Austrian wood flows from the fuzzy set approach (base case) and the least squares approach using the software STAN.

flow	base case	STAN	rel. change
f1	5.15	5.71	-9.5%
f2	2.29	2.40	-4.6%
f3	2.32	2.17	6.9%
f4	0.78	0.68	14.1%
f5	1.30	1.25	4.0%
f6	0.18	0.18	0.6 %
f7	1.07	1.26	-15.0%
f8	0.82	0.90	-8.6%
f9	1.28	1.49	-14.3%
f10	0.18	0.17	3.3%
f11	1.46	1.48	-1.27%
f12	0.03	0.02	20.2%
f13	0.43	0.44	-2.7%
f14	0.38	0.39	-2.5%
f15	0.18	0.18	-1.5%
f16	0.10	0.10	4.5%
f17	0.16	0.15	8.4%
f18	0.17	0.17	2.67%
f19	0.86	0.59	45.2%
f20	0.85	0.73	15.7%
f21	1.53	1.29	18.5%
f22	0.16	0.16	2.7%
f23	0.04	0.08	-50.6%
f24	0.06	0.06	-5.6%
f25	0.04	0.04	-0.6%
f26	0.29	0.30	-3.0%

6 SI-6: Reconcilation algorithm for the base case in Matlab

6.1 Uncertainty characterisation

Data uncertainty characterisation is presented on two overdetermined flows; f11 is an example for homogeneous data points and f23 for heterogeneous ones. Uniquely defined flows are determined by analogy to homogeneous data points with one data point and ucertainty range instead of the average of two.

```
% f11 (homogeneous data points)

%data points and uncertainty ranges
val1=mean(2.4 2.6); %mean of data points of quantity
val2=0.69;     %data point of conversion factor
lev1=0.148;   %mean of share of uncertainty for quantities
lev2=0.113;  %share of uncertainty for main conversion factor

%determination of supports and cores of fuzzy intervals
a=zeros(1,4);          %quantity
a(1,1)=val1*(1-2*lev1);
a(1,2)=val1*(1-lev1);
a(1,3)=val1*(1+lev1);
a(1,4)=val1* (1+2*lev1);
b=zeros(1,4);      %conversion factor
b(1,1)=0.5;  %data point for possibility of chipboards only
b(1,2)=val2;
b(1,3)=val2;
b(1,4)=val2*(1+2*lev2);

%determination of delta-cuts of membership functions
lin=linspace(0,20,100000);
x=trapmf(lin,a);         %MF of qunatity
y=trapmf(lin,b);         %MF of conversion factor
n=100;
cut1=zeros(n,2);
cut2=zeros(n,2);
delta=zeros(n,1);
delta(1,1)=1;
for j=1:n;
for i=1:length(x)
if(x(i)>=delta(j) && x(i-1)<delta(j))
cut1(j,1)=lin(i);
elseif (x(i)>=delta(j) && x(i+1)<delta(j))
cut1(j,2)=lin(i);
end
end
for i=1:length(y)
if(y(i)>=delta(j) && y(i-1)<delta(j))
cut2(j,1)=lin(i);
elseif (y(i)>=delta(j) && y(i+1)<delta(j))
cut2(j,2)=lin(i);
end
```

```
end
delta(j+1)=delta(j)-0.01;
end

%determination of delta-cuts of flow by multiplication
%of delta-cut values of quantity & conversion factor
cut=zeros(n,2);
for j=1:n
cut(j,1)=cut1(j,1)*cut2(j,1);
cut(j,2)=cut1(j,2)*cut2(j,2);
end
cut(1,:)=[cut1(1,1)*b(2),cut1(1,2)*b(3)];
cut11=[cut;[a(1)*b(1),a(4)*b(4)]];


% f23 (heterogeneous data points)

%data for f23a
val1=2.814; % aggregated quantity
val2=0.11;   % fraction of share
lev1=0.22;  %share of uncertainty of quantity
lev2=0.22;  %share of uncertainty of fraction share

%determination of share of quantity
a=zeros(1,4);
b=zeros(1,4);
a(1,1)=val1*(1-2*lev1);
a(1,2)=val1*(1-lev1);
a(1,3)=val1*(1+lev1);
a(1,4)=val1*(1+2*lev1);
b(1,1)=val2*(1-lev2);
b(1,2)=val2;
b(1,3)=val2;
b(1,4)=val2*(1+2*lev2);
lin=linspace(0,20,100000);
x=trapmf(lin,a);
y=trapmf(lin,b);
n=100;
cut1=zeros(n,2);
cut2=zeros(n,2);
delta=zeros(n,1);
delta(1,1)=1;
for j=1:n;
for i=1:length(x)
if(x(i)>=delta(j) && x(i-1)<delta(j))
cut1(j,1)=lin(i);
elseif (x(i)>=delta(j) && x(i+1)<delta(j))
cut1(j,2)=lin(i);
end
end
for i=1:length(y)
if(y(i)>=delta(j) && y(i-1)<delta(j))
cut2(j,1)=lin(i);
elseif (y(i)>=delta(j) && y(i+1)<delta(j))
cut2(j,2)=lin(i);
end
end
```

```
delta(j+1)=delta(j)-0.01;
end
cut=zeros(n,2);
for j=1:n
cut(j,1)=cut1(j,1)*cut2(j,1);
cut(j,2)=cut1(j,2)*cut2(j,2);
end
cut(1,:)=[cut1(1,1)*b(2),cut1(1,2)*b(3)];
cut=[cut;[a(1)*b(1),a(4)*b(4)]];


%conversion of share of quantity into tons dry matter
fuzzy=[cut(101,1),cut(1,1),cut(1,2),cut(101,2)];
a=fuzzy;                                    %share of quantity
val2=0.43;       %conversion factor data point
lev2=0.4395;  %share of uncertainty  of conversion factor
b=zeros(1,4);
b(1,1)=val2*(1-lev2);
b(1,2)=val2;
b(1,3)=val2;
b(1,4)=val2*(1+lev2);
lin=linspace(0,20,100000);
x=trapmf(lin,a);
y=trapmf(lin,b);
n=100;
cut1=zeros(n,2);
cut2=zeros(n,2);
delta=zeros(n,1);
delta(1,1)=1;
for j=1:n;
for i=1:length(x)
if(x(i)>=delta(j) && x(i-1)<delta(j))
cut1(j,1)=lin(i);
elseif (x(i)>=delta(j) && x(i+1)<delta(j))
cut1(j,2)=lin(i);
end
end
for i=1:length(y)
if(y(i)>=delta(j) && y(i-1)<delta(j))
cut2(j,1)=lin(i);
elseif (y(i)>=delta(j) && y(i+1)<delta(j))
cut2(j,2)=lin(i);
end
end
delta(j+1)=delta(j)-0.01;
end
delta=delta(1:100,:);
cut=zeros(n,2);
for j=1:n
cut(j,1)=cut1(j,1)*cut2(j,1);
cut(j,2)=cut1(j,2)*cut2(j,2);
end
cut(1,:)=[cut1(1,1)*b(2),cut1(1,2)*b(3)];
cut=[cut;[a(1)*b(1),a(4)*b(4)]];
delta=[delta;0];
delta2=delta(101:-1:1);
f=[delta2',delta'];
```

```
cutinv=cut(101:-1:1,1);
z=[cutinv',cut(:,2)'];
[C,iz,ic]=unique(z);
f2=f(iz);
zq=0:0.0001:20;
vq1=interp1(C,f2,zq);
cut23a=cut;     %delta-cuts for f23a
f23a=vq1;        %interpolated MF

%data for f23b
val1=0.03;   %quantity in tons
lev1=0.491;  %share of uncertainty

%determination of f23b
a=zeros(1,4);
a(1,1)=val1*(1-2*lev1);
a(1,2)=val1*(1-lev1);
a(1,3)=val1*(1+lev1);
a(1,4)=val1*(1+2*lev1);
lin=linspace(0,20,100000);
x=trapmf(lin,a);
n=100;
cut=zeros(n,2);
delta=zeros(n,1);
delta(1,1)=1;
for j=1:n;
for i=1:length(x)
if(x(i)>=delta(j) && x(i-1)<delta(j))
cut(j,1)=lin(i);
elseif (x(i)>=delta(j) && x(i+1)<delta(j))
cut(j,2)=lin(i);
end
end
delta(j+1)=delta(j)-0.01;
end
delta=delta(1:100,:);
cut=[cut;[a(1),a(4)]];
delta=[delta;0];
delta2=delta(101:-1:1);
f=[delta2',delta'];
cutinv=cut(101:-1:1,1);
z=[cutinv',cut(:,2)'];
[C,iz,ic]=unique(z);
f2=f(iz);
zq=0:0.0001:20;
vq1=interp1(C,f2,zq);
cut23b=cut;  %delta-cuts of f23b
f23b=vq1;    %interpolated MF

%data fusion of f23a and f23b into one MF
n=length(vq1);
TF1=isnan(f23a);
TF2=isnan(f23b);
for i=1:n
if TF1(i)==1
f23a(i)=0;
end
```

```
end
for i=1:n
if TF2(i)==1
f23b(i)=0;
end
end
sum=zeros(1,n);
for i=1:n
sum(i)=f23a(i)+f23b(i); %sum of MFs
end
l=length(sum);
s=zeros(1,l);
for j=1:l
s(j)=sum(j)/max(sum); %normalisation
end

%transformation of MF for f23 into delta-cuts
cut=zeros(101,2);
for j=2:100;
for i=1:length(s)
if(s(i)>=delta(j) && s(i-1)<delta(j))
cut(j,1)=zq(i);
break
end
end
for i=length(s):-1:1
if (s(i)>=delta(j) && s(i+1)<delta(j))
cut(j,2)=zq(i);
break
end
end
end
for i=1:length(s)
if s(i)>0
cut(101,1)=zq(i);
break
end
end
for i=length(s):-1:1
if s(i)>0
cut(101,2)=zq(i);
break
end
end
for i=1:length(s)
if s(i)==1
cut(1,1)=zq(i)
break
end
end
for i=length(s):-1:1
if s(i)==1
cut(1,2)=zq(i)
break
end
end
cut23=cut;
```

6.2 Balancing of the model and data

The data reconciliation consists of 3 steps: balancing of the internal flows, updating the balance constraints with the reconciled internal flows and finally, balancing of the external flows. This is shown on the example of the building industry process. The internal flows are f8 and f16, reconciliation is shown on the example of f8.

```
%building industry constraint:
%delta-cuts given from uncertainty characterisation in 2.1.:
cut8;cut11;cut12;cut13;cut14;cut15;cut16;cut17;cut18;

2.2.1.Determination of constraint intervals f. internal flows

%solutions for f8 and f16 out of balance constraint
BCcut8B=zeros(101,2);  %2nd balance constraint for flow8
BCcut16=zeros(101,2);  %1st balance constraint for flow16
for i=1:101
BCcut8B(i,1)=cut11(i,1)+cut12(i,1)+cut16(i,1)+cut17(i,1)+
+cut18(i,1)-cut13(i,2)-cut14(i,2)-cut15(i,2);
BCcut8B(i,2)=cut11(i,2)+cut12(i,2)+cut16(i,2)+cut17(i,2)+
+cut18(i,2)-cut13(i,1)-cut14(i,1)-cut15(i,1);

BCcut16(i,1)=-cut11(i,2)-cut12(i,2)-cut17(i,2)-cut18(i,2)+
+cut8(i,1)+ cut13(i,1)+cut14(i,1)+cut15(i,1);
BCcut16(i,2)=-cut11(i,1)-cut12(i,1)-cut17(i,1)-cut18(i,1)+
+cut8(i,2)+ cut13(i,2)+cut14(i,2)+cut15(i,2);
end


2.2.2.Determination of internal flows

%assumption: delta-cut for f8 calculated from sawing ind.
%process constraint  (step 2.2.1.) is given
BCcut8;

%intersection of results of both balance constraints
cutA=BCcut8;
cutB=BCcut8B; %from 2.2.1 (building industry process)
cut=zeros(101,2);
delta=[1:-0.01:0]';
level=0;
sol=ones(1,1);
z=zeros(1,2);
for j=1
A=0;
B=0;
C=0;
D=0;
interval=0;
i=101;
while(sol(j)~=0 && i>=1)
A=cutA(i,2*j-1);
B=cutA(i,2*j);
C=cutB(i,2*j-1);
D=cutB(i,2*j);
```

```
if (C>=B || A>=D)
sol(j)=0;
else
X=A:0.0001:B;
Y=C:0.0001:D;
interval=intersect(round(1e4*X)/1e4,round(1e4*Y)/1e4);
z(j,1)=min(interval);
z(j,2)=max(interval);
cut(i,2*j-1)=min(interval);
cut(i,2*j)=max(interval);
level(j)=delta(i);
i=i-1;
end
end
end
BCcut8X=cut(1:101,1:2);
level1=level;                    %level of intersection
unnormed=BCcut8X;
unnormed=unnormed(i+1:1:101,1:2); %intersected interval of constraints

%intersection of intersected constraint interval & input data interval
input=cut8; %from uncertainty characterisation
input=input(i+1:1:101,1:2); %up to previous intersection level
cutA=unnormed; %from BC intersection
cutB=input;
l=length(unnormed);
cut=zeros(l,2);
delta2=delta(101:-1:1);
level=0;
sol=ones(1,1);
z=zeros(1,2);
for j=1
A=0;
B=0;
C=0;
D=0;
interval=0;
i=l;
while(sol(j)~=0 && i>=1)
A=cutA(i,2*j-1);
B=cutA(i,2*j);
C=cutB(i,2*j-1);
D=cutB(i,2*j);
if (C>=B || A>=D)
sol(j)=0;
else
X=A:0.0001:B;
Y=C:0.0001:D;
interval=intersect(round(1e4*X)/1e4,round(1e4*Y)/1e4);
z(j,1)=min(interval);
z(j,2)=max(interval);
cut(i,2*j-1)=min(interval);
cut(i,2*j)=max(interval);
level(j)=level1-(1-delta(i));
i=i-1;
end
end
```

```
end
cut=[zeros((101-1),2);cut];
cut8X=cut(1:101,1:2);
level2=level;   %final alpha-level of of f8
if (level2<1)  %fixation on the alpha-level-interval up to 1
for j=1:i+1
cut8X(j,:)=cut8X(i+2,:);
end
end

% insert as updated cut8 and updated cut 16 in constraint 3
cut8=cut8X;
cut16=cut16X; %assumed to be given, calc. on analogy to cut8X

%solutions for external flows out of balance constraints
BCcut19=zeros(101,2);
BCcut20=zeros(101,2);
BCcut21=zeros(101,2);
BCcut22=zeros(101,2);
for i=1:101
BCcut19(i,1)=cut20(i,1)+cut21(i,1)+cut22(i,1)-cut9(i,2)-cut16(i,2);
BCcut19(i,2)=cut20(i,2)+cut21(i,2)+cut22(i,2)-cut9(i,1)-cut16(i,1);

BCcut20(i,1)=cut9(i,1)+cut16(i,1)+cut19(i,1)-cut21(i,2)-cut22(i,2);
BCcut20(i,2)=cut9(i,2)+cut16(i,2)+cut19(i,2)-cut21(i,1)-cut22(i,1);

BCcut21(i,1)=cut9(i,1)+cut16(i,1)+cut19(i,1)-cut20(i,2)-cut22(i,2);
BCcut21(i,2)=cut9(i,2)+cut16(i,2)+cut19(i,2)-cut20(i,1)-cut22(i,1);

BCcut22(i,1)=cut9(i,1)+cut16(i,1)+cut19(i,1)-cut20(i,2)-cut21(i,2);
BCcut22(i,2)=cut9(i,2)+cut16(i,2)+cut19(i,2)-cut20(i,1)-cut21(i,1);
end


2.2.3. Final reconciliation (of external flows)

%assumption: given in advance
cut A;   %all flows from input data
cutB;    % BC results out of 2.2 for all constraints

%determination of final matrix with all flows intersected
% (no changes happen for the internal flows)
cut=zeros(101,52);
level=zeros(26,1);
sol=ones(26,1);
z=zeros(26,2);
for j=1:26
A=0;
B=0;
C=0;
D=0;
i=101;
while(sol(j)~=0 && i>=1)
A=cutA(i,2*j-1);
B=cutA(i,2*j);
C=cutB(i,2*j-1);
D=cutB(i,2*j);
```

```
if (C>=B || A>=D)
sol(j)=0;
else
X=A:0.001:B;
Y=C:0.001:D;
interval=intersect(round(1e3*X)/1e3,round(1e3*Y)/1e3);
z(j,1)=min(interval);
z(j,2)=max(interval);
cut(i,2*j-1)=min(interval);
cut(i,2*j)=max(interval);
level(j)=delta(i);
i=i-1;
end
end
end
level; %final levels of reconciliation for all flows
cut; %final intervals for all flows

% normalisation of reconciliation to 1
% (so that fuzzy assumptions still hold)
recon=zeros(101,52);
for j=1:26
normed=cut(1:101,2*j-1:2*j);
for k=101:-1:1
if cut(k,2*j-1:2*j)==[0 0]
index=k+1;
break
end
end
normed=normed(index:1:101,1:2);
l=length(normed);
delta2=linspace(0,1,l);
delta2inv=delta2(l:-1:1);
f=[delta2,delta2inv];
normedinv=normed(l:-1:1,1);
z=[normedinv',normed(:,2)'];
zq=0:0.0001:20;
[C,iz,ic]=unique(z);
f2=f(iz);
vq1=interp1(C,f2,zq);
for i=1:length(vq1)
if isnan(vq1(i))==1
vq(i)=0;
end
end
n=100;
recon2=zeros(n,2);
delta=zeros(n,1);
delta(1,1)=1;
for m=1:n;
for i=1:length(vq1)
if(vq1(i)>=delta(m) && vq1(i-1)<delta(m))
recon2(m,1)=zq(i);
elseif (vq1(i)>=delta(m) && vq1(i+1)<delta(m))
recon2(m,2)=zq(i);
end
end
```

```
delta(m+1)=delta(m) - 0.01;
end
recon2=[recon2;[normed(1,1),normed(1,2)]];
recon(1:101,2*j-1:2*j)=recon2;
end
recon;    %final reconciliation results
```

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Article II:
Evaluating the Use of Global Sensitivity Analysis in Dynamic MFA

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Journal of Industrial Ecology, 20 (2016)

Evaluating the Use of Global Sensitivity Analysis in Dynamic MFA

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Keywords:

industrial ecology
material flow analysis (MFA)
parameter uncertainty
sensitivity indices
system dynamics
variance-based sensitivity analysis

Supporting information is linked to this article on the *JIE* website

Summary

Dynamic material flow analysis (MFA) provides information about material usage over time and consequent changes in material stocks and flows. In order to understand the effect of limited data quality and model assumptions on MFA results, the use of sensitivity analysis methods in dynamic MFA studies has been on the increase. So far, sensitivity analysis in dynamic MFA has been conducted by means of a one-at-a-time method, which tests parameter perturbations individually and observes the outcomes on output. In contrast to that, variance-based global sensitivity analysis decomposes the variance of the model output into fractions caused by the uncertainty or variability of input parameters. The present study investigates interaction and time-delay effects of uncertain parameters on the output of an archetypal input-driven dynamic material flow model using variance-based global sensitivity analysis. The results show that determining the main (first-order) effects of parameter variations is often sufficient in dynamic MFA because substantial effects attributed to the simultaneous variation of several parameters (higher-order effects) do not appear for classical setups of dynamic material flow models. For models with time-varying parameters, time-delay effects of parameter variation on model outputs need to be considered, potentially boosting the computational cost of global sensitivity analysis. Finally, the implications of exploring the sensitivities of model outputs with respect to parameter variations in the archetypical model are used to derive model- and goal-specific recommendations on choosing appropriate sensitivity analysis methods in dynamic MFA.

Introduction

Material flow analysis (MFA) is a tool to quantify the flows and stocks of materials in arbitrarily complex systems. Dynamic MFA is a frequently used method to assess past, present, and future stocks and flows of materials in the anthroposphere (Müller et al. 2014). In contrast to static MFA, where material flows are determined for one balancing period and are therefore time independent, material stocks and flows in a dynamic material flow model can potentially depend on all previous states of the system (Baccini and Bader 1996). Recently, dynamic MFA has become increasingly popular, with a primary focus on the investigation of material stocks in society and associated end-of-life (EoL) flows (cf. Laner and Rechberger 2016). Metals, in particular, have been subject to dynamic MFA because of the large accumulated metal stocks in society and their potential value for society as secondary raw materials (cf. Chen and Graedel 2012; Müller et al. 2014).

Given that models represent a simplification of the real metabolic system and because of data limitations in terms of quality and quantity, uncertainty is inherent to material flow analysis (MFA) (Laner et al. 2014). Therefore, uncertainty is a basic aspect of material flow modelling and needs to be explicitly considered to reduce uncertainties and inconsistencies as far as possible, thereby allowing for reliable decision support

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DOI: 10.1111/jiec.12497

Editor managing review: Reinout Heijungs

Volume 00, Number 0

(Gottschalk et al. 2010; Laner et al. 2015). With respect to dynamic MFAs, the in-use stocks and EoL material flows are typically estimated according to a top-down approach (i.e., accounting of the net flows into or out of the stock over time), where substantial uncertainty exists concerning model parameters such as average product lifetimes or historical material-use patterns. Thus, the importance of model calibration and plausibility checks based on independent bottom-up estimates to increase the confidence in dynamic MFA results has been emphasized (Müller et al. 2014; Buchner et al. 2015a).

Sensitivity analysis is carried out to investigate the effect of individual assumptions and parameter specifications on the model output by exploring the effects of the changes of input parameters on the model output. Whereas local sensitivity analysis methods focus on testing different perturbations of constant or uncertain input parameters and analyze the specific consequences in the output, global sensitivity analysis (GSA) focuses on the uncertainty in the output and how it can be apportioned to different sources of uncertainty in the inputs (Saltelli et al. 2008). The process of recalculating outcomes under alternative assumptions to determine the impact of variables using GSA can be useful to identify model inputs that cause significant uncertainty in the output in order to increase robustness of the model and understanding of the relationships between input and output variables (Pannell 1997). Analytical local methods using partial derivatives are usually not useful in dynamic MFA systems given that the model input parameters are uncertain and the model of unknown linearity. Derivatives are only informative in the base point where they are computed and do not provide for an exploration of the rest of the space of input factors, which does not matter for linear systems, but greatly matters for nonlinear ones (Saltelli et al. 2008). Moreover, the global method of regression analysis is typically not a useful option in this context given that it describes only the fraction of linearity within the model output and remains ignorant of the rest of uncertainty or variance within the model (Saltelli et al. 2008). The common way to treat dynamic MFA in previous literature is local, using one-at-a-time (OAT) analysis, where one input variable is changed whereas the others remain fixed in order to see what effect this produces on the output (Murphy et al. 2004). This is very time-consuming if the system consists of many inputs, which need to be observed. Parameter redundancy tests, like the elementary effect test (Morris 1991; Campolongo et al. 2007), can be used to reduce the number of parameters by detecting and excluding those of negligible influence, thereby reducing the input space to be observed. Besides, because materials typically reside for some time in the use phase, input parameters of previous periods affect the uncertainty of the output (in-use stocks, old scrap generation) in later periods. Such time-delay effects are important if model parameters vary over time, which may often be the case in reality (e.g., the share of a material used in a specific application may not be constant over time, but vary because of technological, legal, or socioeconomic changes). Further, OAT analysis cannot account for the combined effects of parameter changes such that interaction effects attributed to the simultaneous variation of parameters are ignored. The standard deviations obtained from the elementary effects test can be used to detect non-monotonic behavior, indicating possible interactions (Garcia Sanchez et al. 2014; Andrianandraina et al. 2015). Because nonlinearities can only be suspected to be interactions (Andrianandraina et al. 2015), further analyses are required also in this case.

Buchner and colleagues (2015a) analyzed the system of Austrian aluminium flows for almost 50 years with time-varying parameters by using variance-based global sensitivity analysis. The analysis focused on the decomposition of the output variance with regard to parts attributable to stochastic input variables and showed that only small parts of the total output variance could be explained by the variation of single parameters in the same year. Thus, more-comprehensive sensitivity analysis approaches are required to investigate the importance of parameter interaction and time-delay effects on the variation of the model outputs.

It is the aim of this study to provide guidance on how to conduct sensitivity analysis in dynamic MFA with regard to the following aspects:

i) How do interaction effects (attributed to simultaneous change of several parameters) influence model results?
ii) How do time-delay effects (influence of parameter values from previous periods on results of subsequent periods) influence model results?
iii) Which problem- and- model-specific recommendations can be given concerning sensitivity analysis in dynamic MFA?

Thereto, the state of the art of sensitivity analysis in dynamic MFAs is reviewed and novel applications of sensitivity analysis are explored. An archetypal dynamic material flow model is established as a highly simplified, reduced version of the national aluminium flow model presented by Buchner and colleagues (2015a) and investigated using a sample-based approach of variance-based GSA. The model contains the essential elements of input-driven top-down dynamic material flow models, which are the distribution of produced materials into different use sectors and the lifetime of products (i.e., in-use stocks) in these sectors (cf. Müller et al. 2014). Based on the analyses, recommendations concerning the choice of sensitivity analysis methods for dynamic MFA are provided.

Sensitivity Analysis in Dynamic Material Flow Analysis

During the last decade, several studies on dynamic MFA considering sensitivity analyses to deal with scenarios or uncertainties within models have been published (see table 1). The first question arising in sensitivity analysis of dynamic MFA is whether the system observation is local or global. Local sensitivity analysis (LSA) aims to highlight changes of the output attributed to certain parameters' perturbations. LSA is mostly an OAT treatment of sensitivity, meaning that single

Table 1 Classification of previous treatment of sensitivity analysis dynamic MFA (based on the review study by Müller et al. 2014)

Classification		
Local SA nominal (1.)	Local SA uncertain (2.)	Global SA (3.)
Dahlström et al. 2004	Zeltner et al. 1999	McMillan et al. 2010
Müller et al. 2006	Spatari et al. 2005	Bader et al. 2011
Geyer et al. 2007	Ruhrberg 2006	Buchner et al. 2015a
Cheah et al. 2009	Gottschalk et al. 2010	
Hirato et al. 2009	Bader et al. 2011	
Chen et al. 2010	Glöser et al. 2013	
Daigo et al. 2010		
Liu et al. 2011		
Müller et al. 2011		
Chen et al. 2012		
Marwede and Reller 2012		
Matsuno et al. 2012		
Liu and Müller 2013a, 2013b		
Pauliuk et al. 2013a, 2013b		

Note: SA = sensitivity analysis.

parameters are tested individually for their sensitivities, but also groups of parameters can be tested together for their sensitivities. There are also local sensitivity analyses that consider parameters as uncertain. Whereas LSA tries to explain the impacts by changing model parameters, GSA starts the analysis from the uncertainty in the output. GSA looks for the highest variations of the output by exploring the whole space of input parameters. Hence, in contrast to LSA, GSA always considers uncertain input parameters. Overall, the treatment of sensitivity analysis in dynamic MFA can be categorized into three groups:

(1) LSA with nominal parameters (LSAn), testing the perturbations of single parameters on the output and comparing them to the baseline scenario.
(2) LSA with uncertain parameters (LSAu), observing the impact of the parameters' uncertainty on the uncertainty of the output.
(3) GSA, explaining how the whole uncertainty of an output can be apportioned to different sources of uncertainties in the input parameters (Saltelli et al. 2008).

LSAn and LSAu use specific, previously determined input parameters to analyze the model output, which are either of general relevance or specifically interesting because of the expert's knowledge of the system. Although parameter uncertainty may be treated within the dynamic model, LSAn ignores the issue when testing the sensitivities by representing the parameters as nominal values. The usual uncertainty treatment in LSAu and GSA is by expressing input parameters as probability density functions.

Most dynamic MFA studies use LSAn by arbitrarily choosing specific parameters, which are changed one at a time and the outcome is compared to the baseline result. Examples for OAT analysis applied to dynamic metal flow models on national and global levels are given in table 1.

So far, only a few dynamic MFAs (on metals) apply LSAu, where the sensitivities of the outputs are analyzed through Monte Carlo Simulation (see also table S1 of the supporting information available on the Journal's website). Finally, GSA has hardly been used in dynamic MFAs, with a few notable exceptions.

Bader and colleagues (2011) used a kind of GSA to investigate a copper flow model for Switzerland by focusing on specific stock saturation-based scenarios as the output variation is caused to the extent of 95% by stock saturation. McMillan and colleagues (2010) present a more-specific application of GSA (cf. Müller et al. 2014) to a model on U.S. aluminium stocks and their relationship with economic output. They used a Fourier amplitude sensitivity test (FAST) to identify not only the main, but also interaction effects of parameter variations. However, a limitation of FAST is that it is prone to systematic deviations from the analytical values (bias), which may be attributed to interference problems (Saltelli and Bolado 1998), and is therefore only useful to determine main effects (Saltelli et al. 2008). Buchner and colleagues (2015a) explored the variations in the total scrap output of Austrian aluminium stocks and flows by applying Sobol indices for main effects using the effective algorithm for computing global sensitivity indices (EASI) algorithm (Plischke 2010). The EASI algorithm is, like the FAST algorithm, based on Fourier transformations. However, the application of GSA in Buchner and colleagues (2015a) showed that only small parts of the total variance of old scrap generation could be explained by the variation of single parameters in the same year. Because lifetime functions define the lifetime of materials in in-use stocks, they lead to delayed effects of input parameters on EoL flows. Therefore, in the case of time-varying parameters, sensitivity analysis needs to explicitly account for changes in parameter values over time. Further, the role of interaction effects between parameters on models in dynamic MFAs needs to be illuminated because no studies on such effects in dynamic material flow models have been performed so far (see table S1 of the supporting information on the Web).

In contrast to dynamic MFA studies, sensitivity analysis dealing with time-varying input parameters, as well as interaction effects between parameters, has been applied to the (mathematically) related field of dynamic input-output models. For instance, Ramdani and colleagues (2006) analyzed sensitivities not only for parameters of the same year, but also for past input parameter values using an analytical nonstationary approach for GSA. With respect to parameter interaction patterns, Tøndel and colleagues (2011) presented a hierarchical multivariate regression-based sensitivity analysis avoiding the assumption of parameter independency by clustering input parameters into groups. Both the consideration of the memory effects of previous periods (Ramdani et al. 2006) and the analysis of the total variations of the output, taking into account parameter interactions (Tøndel et al. 2011), are modeling assumptions that should not be ignored in dynamic MFA.

Materials and Methods

Archetypal Dynamic Material Flow Model

Based on existing dynamic material flow models for metals (Buchner et al. 2015a; Liu and Müller 2013a; Pauliuk et al. 2013b), an archetypal model (=reduced model) focusing on the core element of dynamic MFA, namely, the use phase and associated material stocks and EoL flows (cf. Müller et al. 2014), is developed. Material stocks and flows are modeled using an input-driven, top-down approach. Consequently, the predefined material input is distributed to three use sectors with different residence times. The fraction of obsolete material per year of use is defined using Weibull functions, which are widely used to express product lifetimes or failure rates of material components (a comparison on lifetime distribution functions in dynamic MFA is given in Melo [1999]). The sector-split ratios and the average lifetimes are uncertain and expressed as independent normally distributed variables with a relative standard deviation of 10%. The model output of interest is the old scrap flow (output from the use phase), where the total output O(t) consists of EoL flows from sector 1 $O_1(t)$, sector 2 $O_2(t)$, and sector 3 $O_3(t)$ (see figure 1 and equation 1). The model output for each time period t is obtained by the following convolution formula:

$$O(t) = \sum_{i=1}^{3} O_i(t) = \sum_{i=1}^{3}\sum_{\tau=0}^{t} r_i(\tau)\, l_i(t-\tau)\, I(\tau)\, d\tau \qquad t = \{1, 2, \ldots, T\} \tag{1}$$

In equation (1), T denotes the time range of the system observation, I(t) denotes the input in the period t, $r_1(t)$, $r_2(t)$, and $r_3(t)$ the three sector split ratios in period t, with the corresponding average lifetimes $l_1(t)$, $l_2(t)$ and $l_3(t)$. τ is the time the material input enters the specific sector, taking values between 1 and t. The mean values of the probability density functions of the sector split ratio parameters are denoted as m_{r1}, m_{r2}, and m_{r3} and the means of the average lifetime probability density functions as m_{l1}, m_{l2}, and m_{l3}.

The Weibull probability density function is described in equation (2) as a function of τ (time of input entering use) and two model parameters (the average lifetime l_i and the scale parameter z).

$$wblpdf\,(\tau \mid l_i, z) = \frac{z}{l_i}\left(\frac{\tau}{l_i}\right)^{z-1} e^{-\left(\frac{\tau}{l_i}\right)^{z}} \qquad \tau = \{1, 2, \ldots, t\}, \quad i = \{1, 2, 3\}. \tag{2}$$

The normally distributed average lifetimes $l_1 l_2$,l_3 characterize scale parameters, and z is responsible for the shape of the Weibull probability density function. Here, $z = 3$ is used in accord with Buchner and colleagues (2015a) (based on Chen et al. [2012], Dahlström et al. [2004], Liu and Müller [2013a], and Melo [1999]).

The variance in the old scrap is an aggregation of the variances of the uncertainty within input parameters. The reduced model is subsequently used to study how the total variance of the old scrap output (EoL material flow) can be properly apportioned into the uncertainty of the varying input parameters over time and which changes in input parameters affect the variance of output most in which time period.

Scenario Analysis

Different model setups (=scenarios) are used to analyze interaction and time-delay effects on the model output (see table 2). In scenario 1, the counteracting effects of lifetime and sector split ratio are explained by means of the sector output O_2. This scenario is important in order to understand further ones. Scenario 2 expands the analysis to the full system output by observing all lifetime and sector split ratio effects at once and comparing this for a linear and a constant input over time. For both scenarios, the parameters are stationary over time. In scenario 3, the parameter effects are observed for a specific year of output whereby time-varying parameters are compared to stationary ones. This is under the assumption that input is constant over time. The allocation of the scenarios with regard to the main drivers is given in table 2.

Effect of Time-Independent Parameters on the Output Over Time

In this case, the effects of changes in time-independent parameters (i.e., constant over time) on the outputs are explored throughout the modeling period T = 50 years in scenario 2 (and T = 100 years for relationship analyses in scenario 1) to investigate time-delay effects of parameters' variations on the output. The mean values for the sector split ratios and the corresponding mean values of the average lifetimes are given in

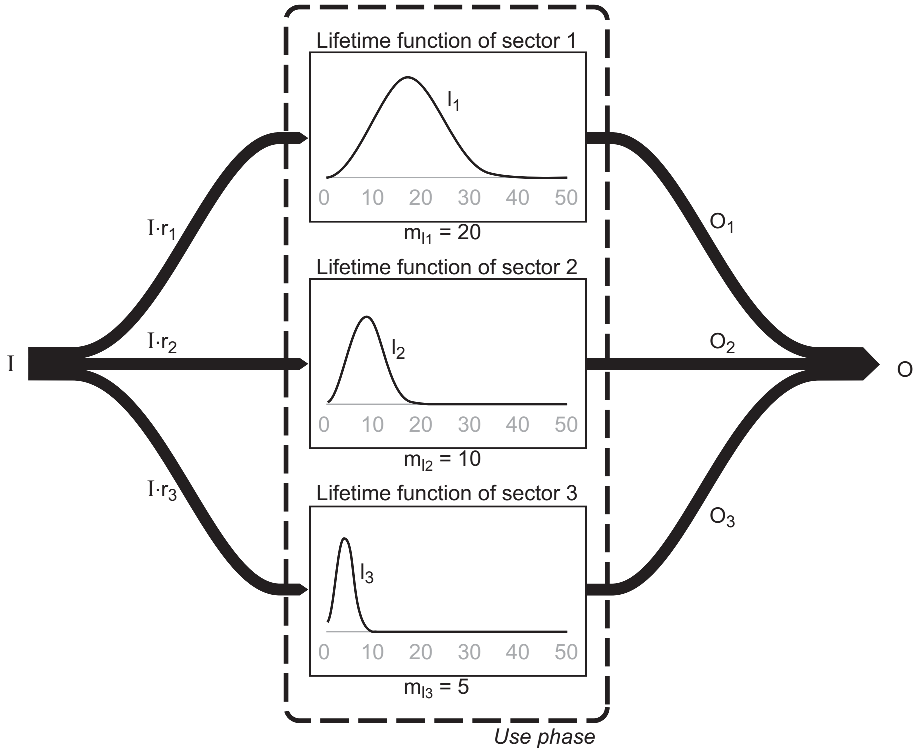

Figure 1 Schematic illustration of the reduced dynamic material flow model, consisting of three in-use sectors with specific lifetimes. The input (I) is split into the use sectors according to the split ratios r_1, r_2, and r_3 and the sector-specific mean average lifetimes given by m_{l1}, m_{l2}, and m_{l3}; O denotes output.

table 2. Because of the residence time of materials in use, the inputs of the three sectors enter the total output with a time delay. Therefore, changes in those inputs can affect the output at any later time given that the time of outflow is random. In scenario 2, the system is tested for different inputs as a model driver, for a constant input and a linearly growing input (see table 2), which is similar to the aluminium input growth in Buchner and colleagues (2015a).

Effect of Time-Dependent Parameters on the Output of a Specific Year

In the case of time-independent parameters, effects of parameter variation on the output are accumulated and it is not possible to trace the individual contribution of input parameters from specific previous years to the output in a certain year. Therefore, the next step is to investigate the sensitivity of output in a specific year with respect to time-dependent parameters (i.e., different values for different time periods). This represents a frequently occurring situation in dynamic material flow modeling when current in-use stocks and old scrap flows are calculated from historical data. The effects of previous parameters were tested for the output in year 50 in scenario 3. In order to compare time varying with stationary parameters, parameters were defined for three time periods. During these periods, the parameter values remain constant, leading to step-wise changes and resulting in 18 input variables in total. The first period denotes the value of the parameters during years 1 to 16 of input. In this phase, both versions have the same parameter values, which are the ones assumed before (see table 2). Whereas for the stationary case the parameters were redrawn with the same mean values for the other two periods, the time-varying parameters rise or fall in two steps, in the second period during years 17 to 33 and the third period from year 34 to observed year of output (which is 50). The changes in sector split parameters sum up to 1 in each of the three periods. The material input per year is given for 50 years (see table 2). A practical example for the first sector, where the mean ratio m_{r1} rises and, simultaneously, the lifetime rises, would be the aluminium use in vehicles (cf. Buchner et al. 2015b).

Variance-Based Sensitivity Analysis

We use variance-based sensitivity analysis to find out how the variance of the output over time can be decomposed into the conditional variances caused by the input parameters from the current and previous periods. We are interested not only in the single effects, but also in the interaction effects originating from combined effects of input parameters $p_1, \ldots, p_k$ on the output $Y = f(p_1, \ldots, p_K)$.

The total or unconditional variance of the output $V(Y)$ is an aggregated sum of all conditional variances of the output. However, it can be restricted to one or combinations of parameters. The normalized partitions of these conditional variances are denoted as sensitivity indices. Three kinds of sensitivity indices

Table 2 Scenario overview about the scenario motivation, input definition, observed output, and chosen mean parameter values

Scenario	*Observation*	*Shape of input curve*	*Input and output observation*	*Values of parameters*
1	*Explanation of counteracting effects of lifetimes and sector split ratios on the example on the single output O_2*	*Constant*	*Input over 50 years, Output observed for 100 years*	*Stationary over time* *Parameter* m_{r2}: 0.3 m_{l2}: 10
2	*The total output O, consisting of three different sectors is analysed with respect to the effect of varying lifetimes and sector split ratios*	*Constant and linearly increasing*	*Input over 50 years, Output observed for 50 years*	Stationary over time *Parameter* m_{r1}: 0.5 m_{r2}: 0.3 m_{r3}: 0.2 m_{l1}: 20 m_{l2}: 10 m_{l3}: 5
3	*The output in year 50 is observed for a) stationary and b) time-varying parameter effects (three previous periods)*	*Constant*	*Input over 50 years, Output of year 50 is investigated (importance of parameter changes in previous periods)*	*Stationary parameters same as in Scenario 2 for all periods; Time-varying parameters:* *Period / Parameter*: *1*, *2*, *3* m_{r1}: *0.5*, *0.6*, *0.7* m_{r2}: *0.3*, *0.25*, *0.2* m_{r3}: *0.2*, *0.15*, *0.1* m_{l1}: *20*, *30*, *40* m_{l2}: *10*, *7.5*, *5* m_{l3}: *5*, *10*, *15*

are considered (Saltelli et al. 2008, chapter 4) (equations 3, 4, and 5):

$$S_i = \frac{V(E(Y|p_i))}{V(Y)} \quad \text{First order effect of parameter i} \tag{3}$$

$$S_{Ti} = 1 - \frac{V((Y|p_{\sim i}))}{V\ (Y)} \quad \text{Total order effect of parameter } i \tag{4}$$

$$S_{Hi} = S_{Ti} - S_i \quad \text{Higher order effect of parameter i } (i = 1,.., n) \tag{5}$$

The nominator in equation (3), $V(E(Y \mid p_i))$, is the expected reduction in variance that would be obtained by fixing p_i. Because the total variance can be decomposed, it holds that $V(E(Y \mid p_i)) + E(V(Y \mid p_i)) = V(Y)$ (Saltelli et al. 2008, chapter 4). In equation (4), $E(V(Y \mid p_{\sim i}))$ is the expected variance that would be left by fixing all factors but p_i. This holds because $V(E(Y \mid p_{\sim i}))$ is the expected reduction in variance obtained by varying all factors but p_i and $V(E(Y \mid p_{\sim i})) + E(V(Y \mid p_{\sim i})) = V(Y)$ (Saltelli et al. 2008 chapter 4 2009).

The first order effect S_i given in equation (3) is the impact on the variance of the output of a parameter alone, whereas the higher-order effect S_{Hi} in equation (5) gives all the combined effects of a parameter with other parameters. The total-order effect S_{Ti} (equation (5)) is all kinds of impact on the output's variance caused by a parameter, alone and in combination with other parameters. As the conditional variances are normalized, they sum up to 1. Thus, the sum of S_i is smaller than 1 in general. The sum of S_i is equal to 1 if there are no interaction effects in the model, which means that S_{Hi} is equal to 0. In this case, the sum of S_{Ti} is also 1. In general, the sum of the S_{Ti} is greater than 1 because potentially present interaction effects are counted multiple times.

To obtain the conditional variances, random drawings are needed to estimate the inner expectation $E(Y \mid p_i)$ for a fixed value of each input variable p_i, and then different values of p_i to estimate the outer variance $V((E(Y \mid p_i))$. Single, combined, and total effects of each year were calculated using Monte Carlo simulations. However, the results can be obtained by a faster short-cut method than doing this for each variable one by one by using a sample-based approach.

Sample-Based Approach

The sample-based computation, based on the procedures presented by Saltelli and colleagues (2008 chapter 4), was conducted as follows:

First, a $X = (N, 2k)$ matrix of random number drawings of the input variables $(p_1, \ldots, p_k)$ is generated, where k denotes the number of parameters and N the order of magnitude, thus the number of Monte Carlo samples. Two matrices A and B of the size (N,k) are defined and each of them contains half of the sample. Next, for each input variable $i = 1, \ldots, k$, a matrix C_i is defined, which contains all columns of B except for the ith column X_i, which is taken from A.

$$A = \begin{bmatrix} x_1^1 & x_2^1 & \ldots & x_i^1 & \ldots & x_k^1 \\ \vdots & & \ddots & x_i^2 & & \vdots \\ x_1^N & & \ldots & x_i^N & & x_k^N \end{bmatrix}$$

$$B = \begin{bmatrix} x_{k+1}^1 & x_{k+2}^1 & \ldots & x_{k+i}^1 & \ldots & x_{2k}^1 \\ \vdots & \ddots & & x_{k+i}^2 & & \vdots \\ x_{k+1}^N & \ldots & & x_{k+i}^N & & x_{2k}^N \end{bmatrix}$$

$$C_i = \begin{bmatrix} x_{k+1}^1 & x_{k+2}^1 & \ldots & x_i^1 & \ldots & x_{2k}^1 \\ \vdots & \ddots & & x_i^2 & & \vdots \\ x_{k+1}^N & \ldots & & x_i^N & & x_{2k}^N \end{bmatrix} \quad i = 1, \ldots, k$$

Then, the $N\times1$- outputs are computed for the three input matrices, $y_a = f(A)$, $y_b = f(B)$, $y_{Ci} = f(C_i)$.

The first- and total-order indices are then computed as follows in equation (6) and equation (7):

$$S_i = \frac{V(E(Y|X_i))}{V(Y)} = \frac{y_a * y_{C_i} - f_o^2}{y_a * y_a - f_o^2} = \frac{\left(\frac{1}{n}\right)\sum_{i=1}^{N} y_a^j y_{c_i}^j - f_o^2}{\left(\frac{1}{N}\right)\sum_{i=1}^{N} (y_a^j)^2 - f_o^2}. \tag{6}$$

$$S_{T_i} = 1 - \frac{V(E(Y|X{\sim}_i))}{V(Y)} = 1 - \frac{y_b * y_{C_i} - f_o^2}{y_a * y_a - f_o^2} = 1 - \frac{\left(\frac{1}{n}\right)\sum_{i=1}^{N} y_b^j y_{c_i}^j - f_o^2}{\left(\frac{1}{N}\right)\sum_{i=1}^{N} (y_a^j)^2 - f_o^2}. \tag{7}$$

with $f_0^2 = (\frac{1}{N}\sum_{j=1}^{N} y_a^j)^2$.

Picking out one of the scalar products of the different matrix-outputs $y_a * y_{C_i}$, all factors of the output Y computed from the inputs from A are resampled, except for the values in column X_i (the drawn samples of parameter p_i), which remain fixed. Hence, if X_i is noninfluential, then high and low values of y_a and y_{C_i} are randomly associated so that they balance out. If X_i is influential, high values of y_a are then multiplied with high values of y_{C_i} and low ones of y_a with low ones of y_{C_i}, which increases the resulting scalar product. The same idea holds for the product of the first-order effects of non-X_i $y_b * y_{C_i}$ (Saltelli et al. 2008, chapter 4).

The resulting first-order indices of the sample-based approach (see equation 6) are checked against first-order indices S_i derived using variance decomposition methods based on Fourier transformations. Such algorithms are suitable to determine main parameter effects computationally more efficient than the sample-based approach described above. In this study, the EASI algorithm (Plischke 2010), which belongs to the class of FAST Fourier transformations, is used for evaluating the plausibility of first-order indices and testing their convergence (see section S2 in the supporting information on the Web).

Results

The results section consists of three subsections dealing with the major findings related to the analysis of three distinct model setups (=scenarios).

Scenario 1: Importance of Lifetime and Sector Split Ratio for Output O_2

The relationship between the sector split ratio of the output and its lifetime follows the same pattern for the first- and total-order indices of each sector: The effects are reverse (see figure 2 for O_2 with the sector split ratio r_2 and average lifetime l_2). The time duration of the growth period, the saturation period, and the degeneration period of the output are influenced by the mean value of the average lifetime, whereas the sector split ratio is responsible for the amount of output. At the beginning, in the growth phase of output, l_2 is significant and r_2 is negligible. This is to be expected because the variation of average lifetime has the sole relevance in terms of the variation of output when almost all input is still kept in stock and the output is low. In the growth phase of output, the average lifetime effect falls whereas the effect of the sector split ratio rises. The sector split ratio is most sensitive to the output during the saturation phase of the output and the average lifetime plays no role in this phase. This is because the effect of the lifetime variations is canceled out through the constant supply of input, that is, higher average lifetime in one year and a lower average lifetime in the following might even out. However, the change in the variation of the sector split ratio would completely change the variation of the output in full. With decreasing output in the degeneration phase, the average lifetime grows and becomes significant again and the importance of the sector split ratio decreases. This is because the less output is given, the more important becomes the time the output flow of a sector enters the output. The higher-order indices become smaller with an increasing number of Monte Carlo samples and are negligible at 100,000 sampling runs. The results of the first-order effects are compared to results obtained by using the EASI algorithm, which are almost identical (see figure S1 of the supporting information on the Web). Besides, for the EASI algorithm, the first-order indices sum up to 1, proofing that there are no higher-order effects.

With respect to dynamic MFA practice, this means that as long as EoL flow volumes are increasing (and the in-use stocks are growing), the uncertainty in average lifetimes is more important than in situations where in-use stocks are closer to saturation or decreasing (and EoL flows also follow a decreasing trend). For the latter kind of situation, the uncertainty associated with sector split ratios comes to the fore when we are interested in determining the EoL flows.

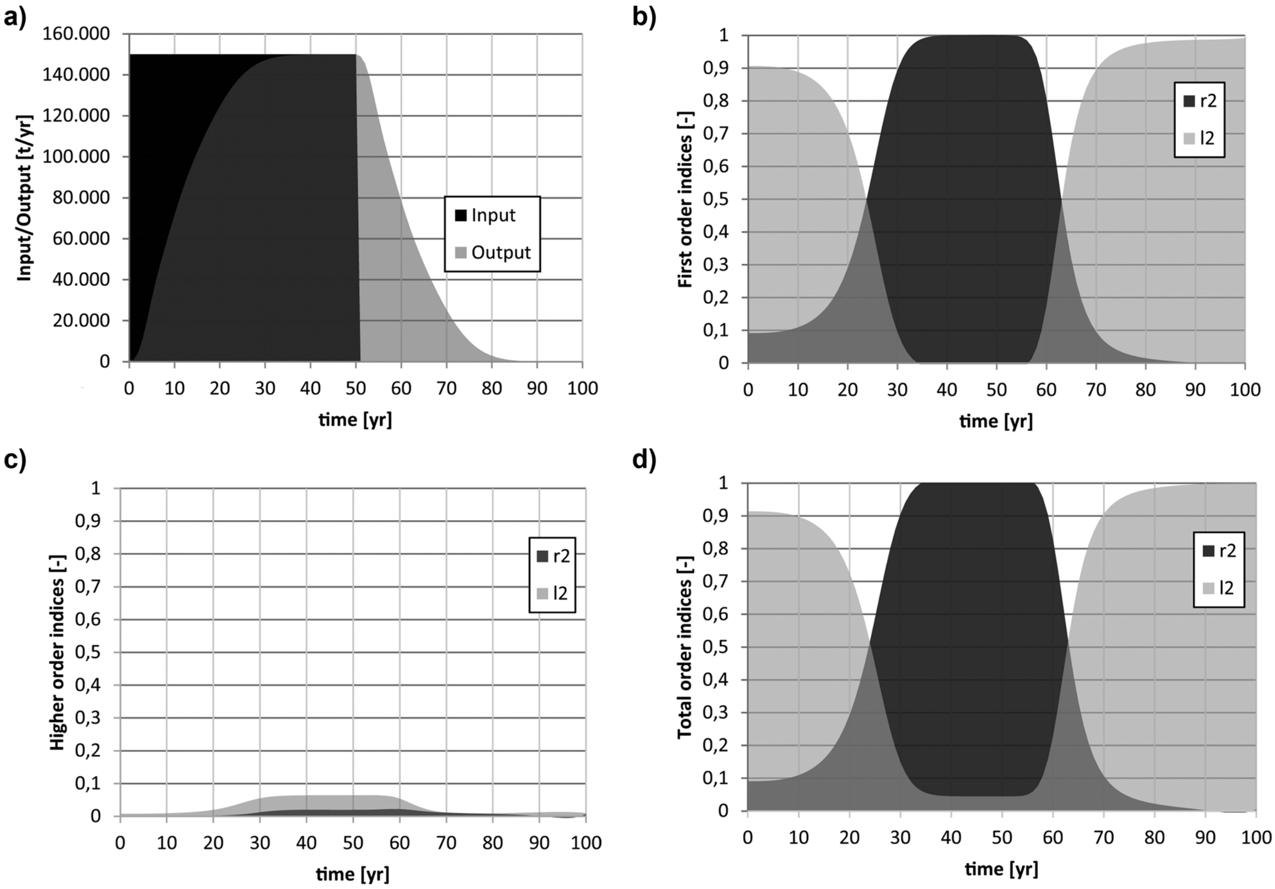

Figure 2 Sensitivity indices for $O_2 = \sum_{\tau=0}^{t} r_2(\tau) l_2(t-\tau) I(\tau) d\tau$. with $m_{r2} = 0.3$ and $m_{l2} = 10$: (a) material input to and output from sector 2, (b) first-order, (c) higher-order, and (d) total-order indices for the sector split ratio and average lifetime of sector 2.
Note: t/yr is tonnes/year, r is split ratio and l is lifetime.

Scenario 2: Sensitivity Analysis of the Total Output O

The dynamic system was tested for a constant input over 50 years and a linearly increasing input over time. The latter has been chosen to resemble typical trends in metal consumption in industrialized countries and is exemplarily based on the increase of aluminium consumption in Austria (see Buchner et al. 2015a). Figure 3 denotes the curve progression of these inputs, the corresponding outputs, and sensitivity indices. When it comes to the order of the most important first- and total-order indices during the period of output, almost all input variations show the same result: In the introduction phase of the output, the shortest average lifetime with $m_{l3} = 5$y is dominant. Then, during the growth phase, the middle average lifetime with $m_{l2} = 10$y dominates all others, and, finally, the longest one with $m_{l3} = 20$y is the most important one. At the beginning of the saturation phase of the output (peak phase for the linear input), the highest sector split ratio with $m_{r1} = 0.5$ becomes significant. Although the effects overlap during the constant input case, the annually growing input and, consequently, also growing output stretches the effects over time.

The constant case shows that all lifetimes are influent in the unstable phase of introduction and the sector split ratios are influent in the stable phase when the output is saturated. The same holds for the linear case; the influencing parameters are the mean average values of lifetimes in the introduction phase and the mean values of the sector split ratios in the saturation phase. The introduction phase is the period of nonlinear behavior of output; thus, the function derivative of the output is growing. The saturation phase is the period where the rate between output and input is practically constant; here, the function derivative of the output is also constant.

The results in figure 3 are obtained after 300,000 Monte Carlo simulation runs. The higher-order indices vary between –0.3 and 0.3 (data not shown). However, negative results are impossible because of mathematical definition and they would vanish with a higher number of simulation runs, which was computationally too expensive in this case. Through computations with a lower number of simulation runs and by observing the sectors individually (cf. scenario 1), it can be seen that the higher-order indices converge toward zero for each case. The results of the first-order effects were compared to the results obtained by the EASI algorithm (see figure S2 of the supporting information on the Web, showing the first-order effects of the same scenario calculated with the EASI algorithm), showing that there are no significant higher-order effects.

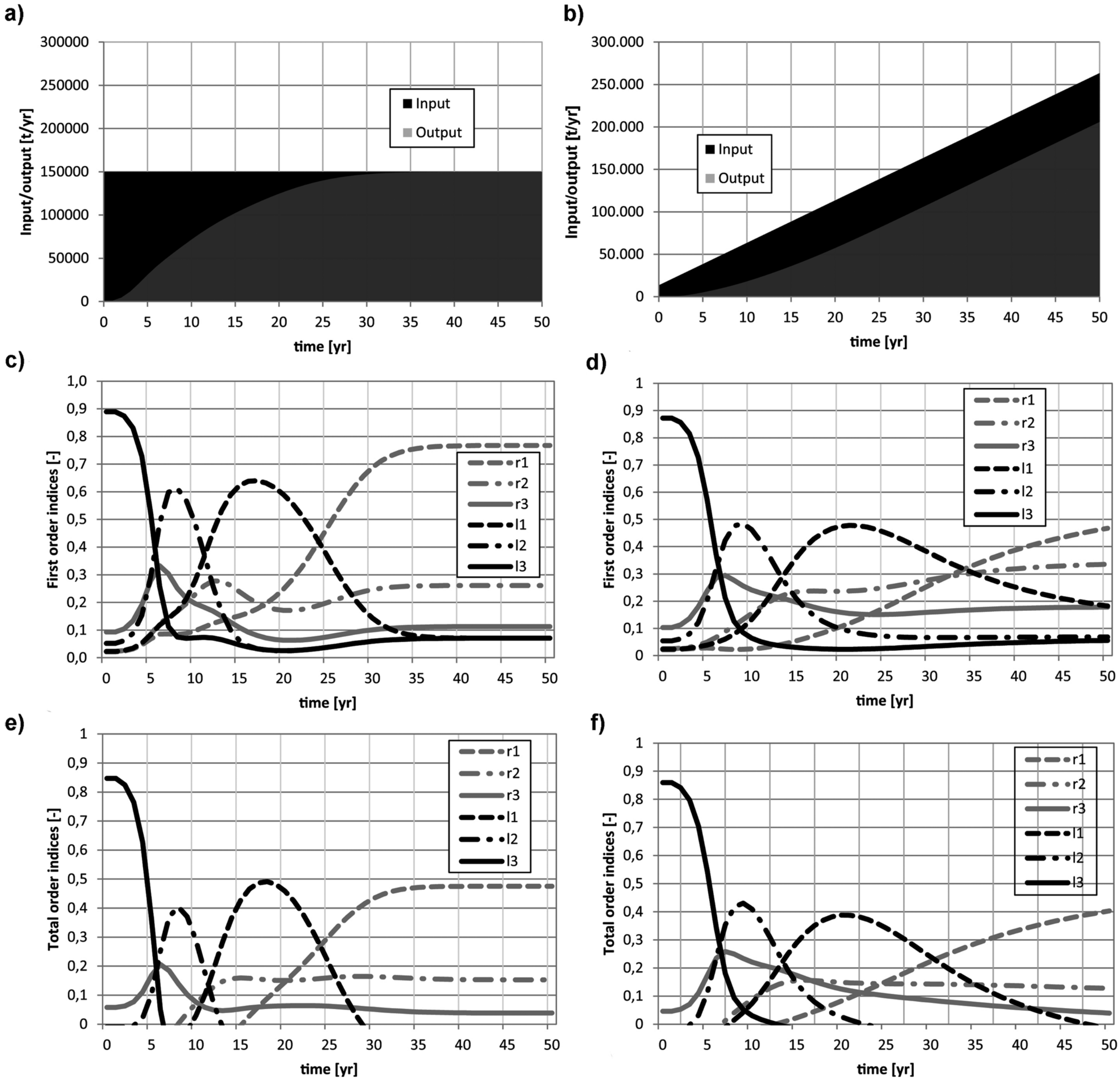

Figure 3 Sensitivity indices for a constant (left column) and a linear (right column) input: illustration of the (a) constant and (b) linearly growing material input and corresponding outputs, (c), (d) the first- and (e), (f) total-order indices for T = 50 years of observation.
Note: t/yr is tonnes/year, r is split ratio, and l is lifetime.

Scenario 3: Parameter Effects on the Output of a Specific Year

The first-order effects show again the same behavior as the total-order effects for both time-varying and stationary parameters. The higher-order effects converge to zero with an increasing number of simulation runs (as can also be seen by the comparison of the first-order effects to those obtained by the EASI algorithm in table S2 of the supporting information on the Web). The effects of the time-varying and stationary parameters over three periods on the output of year 50 are given in table 3. As can be seen in the right bottom corner of table 3a and table 3b, all effects over the three periodical changes sum up to approximately 1 in both cases, meaning that the output variances are fully explained by the first-order indices. All sector split ratios and their corresponding average lifetimes show up at around the same period of time (which is already observed in scenarios 1 and 2). For example, it can be seen that l_1 has the strongest effect in period 2 in both cases. At the same time, r_1 reaches its peak (although the effect is far less than the one of l_1). Obviously, the effects of the sector split ratios of sectors with shorter lifetimes (O_2, O_3) appear close to the year of output 50, whereas the parameters related to O_1 in earlier modeling periods are more important for the output of year 50.

Table 3 First-order indices of the stationary and time-varying parameters for the output in year 50

a) Stationary parameters							
First order indices	r_1	r_2	r_3	l_1	l_2	l_3	*Σ parameters*
Period 1	0.010	0.007	0.005	0.023	0.014	0.009	0.068
Period 2	0.038	0.011	0.011	0.113	0.025	0.012	0.209
Period 3	0.030	0.068	0.083	0.113	0.173	0.311	0.776
Σ periods	0.078	0.086	0.098	0.248	0.212	0.332	1.052

b) Time-varying parameters							
First order indices	r_1	r_2	r_3	l_1	l_2	l_3	*Σ parameters*
Period 1	0.004	0.004	0.004	0.068	0.004	0.004	0.088
Period 2	0.043	0.004	0.004	0.168	0.004	0.004	0.226
Period 3	0.024	0.143	0.021	0.024	0.422	0.062	0.696
Σ periods	0.071	0.151	0.029	0.260	0.430	0.070	1.010

Note: The three periods denote the step-wise changes of parameter values. Period 1: 1 to 16 years; period 2: 17 to 33 years; and period 3: 34 to 50 years. Shades of gray highlight the importance of the parameters in the periods (the darker, the more important).

In both cases, the effects of the first period are negligible given that the average lifetimes (20, 10, and 5 for both) are too short to have an effect on the output in year 50. During years 17 to 33, l_1, the longest average lifetime has the highest and, together with r_1, the dominant effect on the output. Given that a mean average lifetime of $m_{l1} = 30$ in the time-varying case has the highest effect directly in the middle of period 2, this effect is considerably higher than in the stationary case with $m_{l1} = 20$, where the effect is shifted toward the end of period 2 and overlaps with period 3. The shorter the lifetime, the higher is the concentrated effect in one period. This is obvious for period 3, which captures almost 80% of all effects in the stationary case and almost 70% in the time-varying case. Whereas in the stationary case, l_3 is the most important parameter ($m_{l3} = 5$), l_3 is unimportant in the time-varying case, because $m_{l3} = 10$ in period 2 is too short a lifetime to significantly affect the output whereas $m_{l3} = 15$ in period 3 is too long to be an important driver. Apart from that, the sector split ratio of O_3 also decreases to $m_{r3} = 0.1$ ($m_{r3} = 0.2$ in the stationary case) in period 3. In contrast to that, the effect of l_2 is doubled in the time-varying parameters case. Here, m_{l2} shrinks to 5 in the last period ($m_{l2} = 10$ in the stationary case). Because the other average lifetimes do not affect the output directly in this period, this makes l_2 the most important parameter in this case (and r_2 in period 2 the most important sector split ratio). This example shows that changes of parameters over time affect the behavior of sensitivities and lead to nonlinear effects in output dynamics.

Discussion

Reduced Dynamic Material Flow Model

The Sample-Based Approach and Higher-Order Effects

The variance-based sampling method for global sensitivity in dynamic MFA provides a tool to detect not only the main effects, but also interaction effects of the parameters on the variation of output over the periods of observation. The computational effort required of this variance-based method to detect such sensitivity indices is very high, especially if the parameters are observed over a long period of time. Assuming that N denotes the number of Monte Carlo simulation (MCS) runs and k the number of parameters, 2N simulations are needed for computing the outputs of the matrices A and B (y_a and y_b) and kN simulations are needed to compute the k versions of the output of C (y_c). Because all outputs are observed for T years, the cost of the analysis is $m = T(k+2)N$ (cf. Saltelli et al. 2009). In terms of applying the reduced dynamic material flow model, this cost would be 800N for the full system sensitivity analysis.

The patterns of parameter sensitivity in the dynamic systems are already apparent after N = 100,000 MCS runs (m = 80 million). Although the rankings of the first (and total) order indices remain the same, there are still important, observable changes within the sensitivity indices until N = 300,000 runs (calculation time is 3 times higher than for N = 100,000 runs) with m = 240 million.

The higher the number of Monte Carlo runs, the smaller the higher-order indices. Thus, the sensitivity of the model is already fully determined through the first-order indices. This analysis indicates that in such general dynamic MFA cases of combinations of sector split ratios and lifetime functions, higher-order indices are not expected to be significant and can be neglected. Therefore, in these cases, more-efficient algorithms analyzing first-order effects, such as the EASI algorithm, can be used and large numbers of input parameters (like time variations of parameters for each year in this example) can be easily dealt with.

However, there are specific circumstances when higher-order effects may become relevant for sensitivity analysis in dynamic MFA. In such a case, the first-order indices of the parameters do not sum up to unity. For instance, this could be the case for very small material flows, which are distributed into more flows at a later stage of the model. An example would be the material flow out of a very small use sector, which is subsequently directed to a sorting and upgrading plant producing secondary raw materials. Higher-order effects may be relevant for this secondary raw material flow because the probability density function for the respective sector split is located close to zero and several other parameters are multiplied with the sector split ratio to calculate the flow of interest (see figure S3 of the supporting information on the Web). In general, significant parameter interaction effects on the model output may be expected if the output is the product of several variables and (at least) one of the variables is defined in a way that zero lies within the set of probable parameter realizations. It holds that the more often zero is attained within the set of outcomes of the final output, the higher the interaction effects. This is attributed to the fact that if a product has a factor equal to zero, the product becomes zero. A similar relationship may be given for emission flows with low emission factors (see section S3 in the supporting information on the Web). In classical cases, when the observed model output is not a product of many factors with at least one frequently taking zero values, the variation of the output can be explained through the first-order effects over time.

Time-Dependent Parameters and Delayed Effects

The effects of parameters related to inputs to the use phase have a delayed effect on the EoL flows attributed to the use (duration) of materials. Thus, the sensitivity indices of the parameter values also need to be considered with regard to the delay. We showed how sensitivity indices of a set of parameters in the first periods spread over time. However, in most cases, the modeler is interested in finding out which parameters affect the model output for a specific year (e.g., current in-use stocks or old scrap generation). The period of parameter specification needs to be considered if they are time varying. For time-varying parameters, it holds that every change of their probability density function (in our example, the mean value) needs to be considered as a new variable. Here, the appearance of the effects of a sector split ratio and the corresponding lifetime can be approximated by subtracting the average lifetime of the year of observed output. Thus, for short average lifetimes, it holds that the sector split ratios parameters and their corresponding average lifetimes can be neglected in early periods whereas for very long lifetimes, the sector split ratios and their corresponding lifetimes are practically negligible in the years close to the output. Thus, the number of parameters can be reduced to potentially important ones. Otherwise, for instance, in the case of annually changing parameter values, the computational cost of the sample-based approach for sensitivity analysis could become very high. The comparison of stationary and time-varying parameters for a specific year of output shows that the global sensitivity results can differ. If time-varying parameters are treated as stationary in a variance-based sensitivity analysis approach and thus their relative variance is also treated as stationary, the variance of the output is apportioned inconsistently with the actual parameter evolution. In particular, such an allocation is wrong if the parameters vary greatly in size over time.

Recommended Practice for Sensitivity Analysis in Dynamic Material Flow Analysis

When it comes to sensitivity analysis in dynamic MFA, it boils down to the question of which sensitivity analysis approach is appropriate given the model structure and the output of interest.

Considering the previous treatment of sensitivity analysis in dynamic MFA, this approach can expand the classification of sensitivity analysis in two important dimensions: On the one hand, time-delay effects of varying input parameters over the years when in-use stocks are considered and, on the other hand, the observation of interaction effects if dependencies are given (multiplications are done) with values for which the probability density function attains the value zero with high probability (especially if a lot of other parameters depend on this value). The analysis of the dynamic material flow model in this study focused on these two dimensions and showed that:

- For classical dynamic model set ups, higher-order effects do not contribute significantly to the sensitivity of the results.
- EoL flows are sensitive with respect to variations in lifetimes during unstable periods of output, whereas variations in sector split have the dominant effect on EoL flows during stable periods.
- Time-dependent variables need to be checked for delayed effects of previous periods by treating them as separate variables for each significant period of change. A reduction can be made by neglecting parameter values in periods, which are too far off the observed year of output (i.e., if the output in a specific year is of interest for the analysis).

Based on the findings of the sensitivity analysis of the archetypical dynamic material flow model and the review of the current state of the art of sensitivity analysis in dynamic MFA (see section *Sensitivity Analysis in Dynamic Material Flow Analysis*), a recommended practice for sensitivity analysis in dynamic MFA is put forward. The corresponding, hierarchically ordered decision chart with the features of the observed model assumptions and the appropriate sensitivity analysis approach is shown in figure 4.

For systems that do not consider multiplications with parameters for which the probability density function attains zero, a variance-based FAST Fourier transformation algorithm can be used because it is sufficient to determine first-order indices (main parameter effects).

Cases that may have higher-order effects can be solved with the variance-based sampling method or with other methods proposed by Saltelli and colleagues (2009), which are more time efficient. Saltelli and colleagues (2009) proposes Jansen's

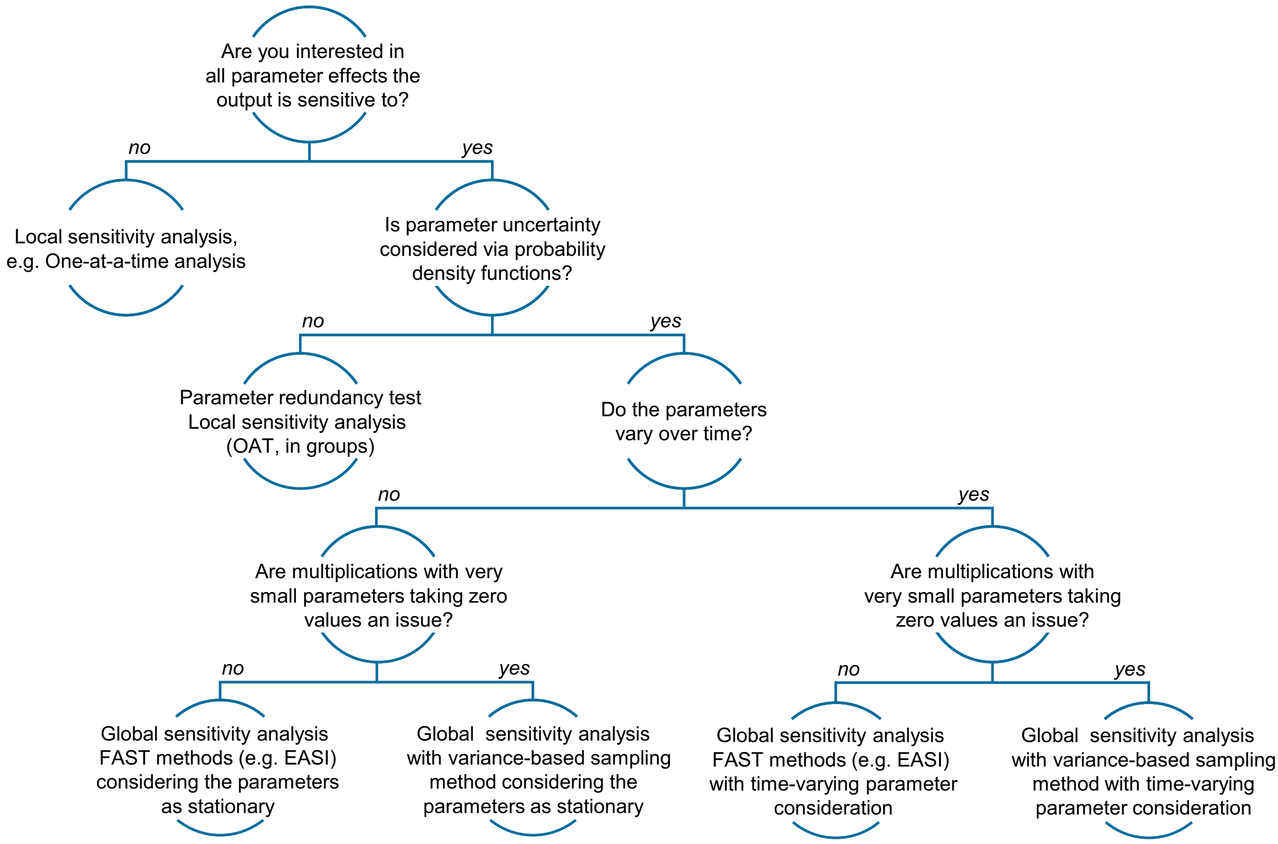

Figure 4 Decision scheme for selecting appropriate methods for sensitivity analysis in dynamic material flow analysis. OAT = one-at-a-time; FAST = Fourier amplitude sensitivity test; EASI = effective algorithm for computing global sensitivity indices.

estimator (Jansen 1999), radial sampling, and a quasi-random number method as the best estimators and as faster alternatives to the sample-based approach for exploring higher-order effects. The choice of method ultimately depends on the goal and scope of the analysis: Is it important to observe the whole system and every output of each time period or is it sufficient to explore the total effects on one output over one or two specific time periods? In the latter case, the variance-based sampling method presented in this article is an appropriate choice.

Dynamic material flow models will gain in complexity in the future attributed to the consideration of various material quality layers (e.g. Buchner et al. 2015b) or the requirement of closed mass balances applied to the model (i.e., recycled material flows have to [exactly] correspond with the quantities used in secondary production). Because higher-order effects are expected to become more prominent in such models, the investigation of parameter interaction effects and parameter dependencies (e.g., Mara et al. 2015) will become a major field for extending the use of sensitivity analysis in dynamic MFA.

Acknowledgments

This research was carried out as a collaborative work within two large-scale research projects: The IRMAR (Integrated Resource Management & Recovery) initiative funded by the Danish Research Council and the Christian Doppler Laboratory on Anthropogenic Resources funded by the Austrian Federal Ministry of Science, Research and Economy and the National Foundation for Research, Technology and Development. Further, financial support by the TU Wien within the program "Innovative Projekte" is gratefully acknowledged.

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Supporting Information

Supporting information is linked to this article on the *JIE* website:

Supporting Information S1: This supporting information contains detailed information about previous topic-related studies using a more-advanced treatment of sensitivity analysis, results for the first-order sensitivity indices in three sections: Section S1 for Scenario 1, Section S2 for Scenario 2, and Section S3 for Scenario 3 using the EASI algorithm (Plischke 2010) and an example on nonzero higher-order effects for a dynamic MFA model.

SUPPORTING INFORMATION FOR:

Dzubur, N., H. Buchner, and D. Laner. 2016. Evaluating the use of global sensitivity analysis in dynamic MFA. *Journal of Industrial Ecology.*

Summary

This supporting information contains detailed information about previous topic-related studies using a more advanced treatment of sensitivity analysis, results for the first order sensitivity indices of in three sections: Section S1 for Scenario 1, Section S2 for Scenario 2, and Section S3 for Scenario 3 using the EASI algorithm (Plischke 2010) and an example on non-zero higher order effects for a dynamic MFA model.

Contents

Section S1: Treatment of sensitivity analysis in dynamic MFA according to different attributes of parameters

Based on a review study by Müller et al. (2014), the use of sensitivity analysis in dynamic MFA is highlighted in **Table S1**.

Table S1: Use of sensitivity analysis in dynamic MFA metal studies (cf. Müller et al. 2014) with regard to different parameter attributes, including the most sophisticated studies with regard to sensitivity analysis

Study	Type of model	Case study	Class	Treatment of parameter uncertainty	Parameter interactions	Stationary/time-varying parameters
Bader et al. 2011	bottom-up	copper	LSAu +GSA	stochastic (PDFs through Gaussian error propagation)	not considered	stationary
Buchner et al. 2015	top-down	aluminium	GSA	stochastic (PDFs)	not considered	time-varying
Cheah et al. 2009	top-down	aluminium	LSAn	none	not considered	stationary
Davis et al. 2007	top-down	iron and steel	LSAn	none	considered	stationary
Glöser et al. 2013	top-down	copper	LSAu	stochastic (PDFs)	not considered	stationary
Gottschalk et al. 2009	top-down	nano-TiO2 particles	LSAu	stochastic (PDFs)	not considered	stationary
McMillan et al. 2010	top-down	aluminium	GSA	stochastic (PDFs)	considered	stationary
Spatari et al. 2005	top-down	copper	LSAu	uncertainty ranges (for average lifetimes)	not considered	stationary

Section S2: Results of first order indices of Scenario 1, 2 and 3 using the EASI algorithm

The EASI algorithm by Plischke (2010) estimates first order sensitivity indices by using Fast Fourier Transformations. The first order results of the scenarios using the sample based approach in section 4 were compared to results obtained by calculating the same scenarios with the EASI algorithm.

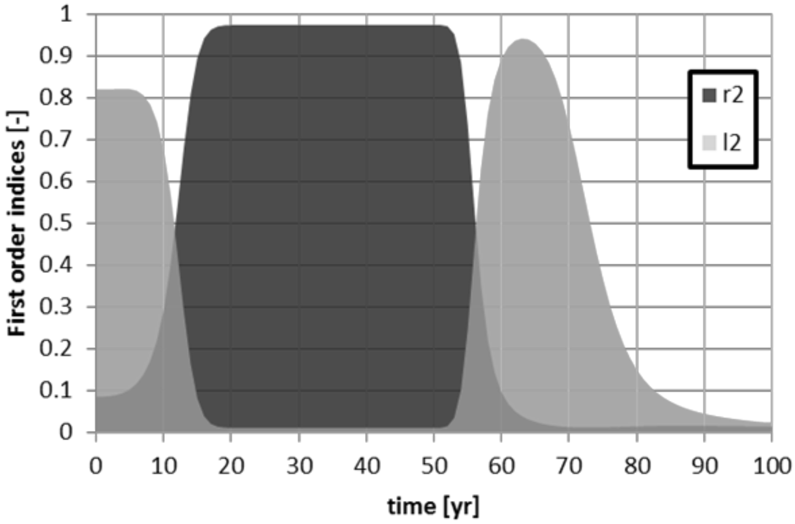

Figure S1: Scenario 1: First order sensitivity indices indices for $O_2 = \sum_{\tau=0}^{t} r_2(\tau) l_2(t-\tau) I(\tau) d\tau$ with mr2=0.3 and ml2=10 for the sector split ratio and average lifetime of sector 2 calculated with the EASI algorithm.

The differences to the first order indices calculated with the sample based approach (see Figure 2) compared to the first order indices obtained by the EASI algorithm in Figure S-1 in the beginning and the end of the time of observation, when output is very small, result of calculation differences.

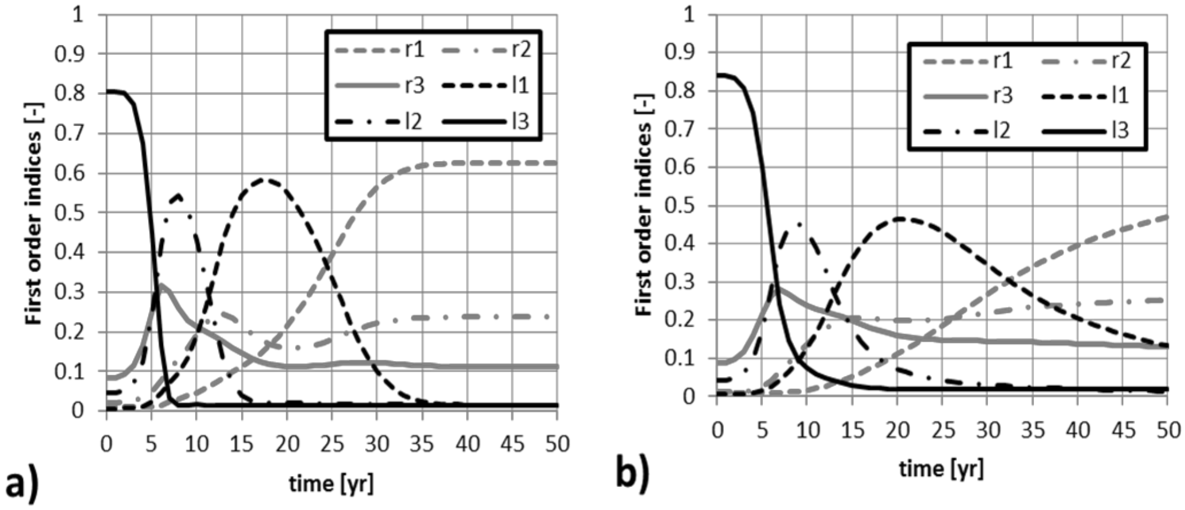

Figure S2: Scenario 2: Sensitivity indices for a constant (a) and a linear (b) input: Illustration of the first order indices for T=50 years of observation using the EASI algorithm.

Table S2: Scenario 3: The first order indices of the stationary (a) and time-varying (b) parameters for the output in year 50 calculated with the EASI algorithm. The three periods denote the stepwise changes of parameter values. Period 1: 1-16 years, Period 2: 17-33 years and Period 3: 34-50 years.

a) Stationary parameters							
First order indices	r_1	r_2	r_3	l_1	l_2	l_3	*Σ Parameters*
Period 1	*0.016*	*0.015*	*0.015*	*0.025*	*0.017*	*0.017*	*0.105*
Period 2	*0.049*	*0.018*	*0.016*	*0.154*	*0.021*	*0.019*	*0.277*
Period 3	*0.045*	*0.066*	*0.060*	*0.154*	*0.184*	*0.202*	*0.711*
Σ Periods	*0.109*	*0.099*	*0.091*	*0.333*	*0.222*	*0.238*	*1.093*

b) Time-varying parameters							
First order indices	r_1	r_2	r_3	l_1	l_2	l_3	*Σ Parameters*
Period 1	*0.025*	*0.018*	*0.018*	*0.028*	*0.018*	*0.015*	*0.121*
Period 2	*0.115*	*0.017*	*0.018*	*0.227*	*0.018*	*0.023*	*0.418*
Period 3	*0.029*	*0.118*	*0.026*	*0.053*	*0.400*	*0.040*	*0.666*
Σ Periods	*0.168*	*0.153*	*0.062*	*0.308*	*0.436*	*0.078*	*1.205*

The calculation results in Table S2 show the same pattern as the sample based approach. However, the numbers are not exactly the same due to the Monte Carlo sampling.

Section S3: Example on higher order effects for a secondary raw material output flow

The following example is a dynamic MFA study, where higher order effects need to be considered in the sensitivity analysis: The output flow is secondary raw material out of a sorting and upgrading plant. A very small use sector with a mean sector split ratio of m_{r1}=0.05 and absolute standard deviation of σ_{r1}=0.05 (the average lifetime has a mean of m_{t1}=20 with σ_{t1}=4) is considered. A fraction so of this sector (m_{so}=0.2, σ_{so}=0.1) is sent to the sorting and upgrading plant and a fraction se (m_{se}=0.8, σ_{se}=0.1) of the latter is used as secondary raw material, see (1).

$$O_{sec\_raw\_mat}(t) = so * se * \sum_{\tau=0}^{t} r_1(\tau) l_1(t-\tau) I(\tau) d\tau \qquad t = \{1,2,\ldots,T=50\}$$

The results in Figure S3 show that higher order effects appear for the secondary raw material output. Their sum varies between 1.9 in the first year and decreases to 0.36 in year 50. While output is growing, the lifetime has the highest first and total order effects and the higher order effects are the highest, as there is no compensation from previous periods and their effects on the output. In the saturation phase, the lifetime effect is balanced out through previous periods. The sector split ratio gets dominant, followed by the sorting fraction so, which are the parameters attaining zero in their ranges. During the saturation phase, they tend to a constant combined effect on the output, while the other parameters are negligible.

A similar relationship as constructed above could apply to emissions into environmental media, which can be determined via emission factors and are often very small (close to zero) as well as highly uncertain. Thus, higher order effects might also play a role in situations when dynamic MFA is used to investigate environmental pollution.

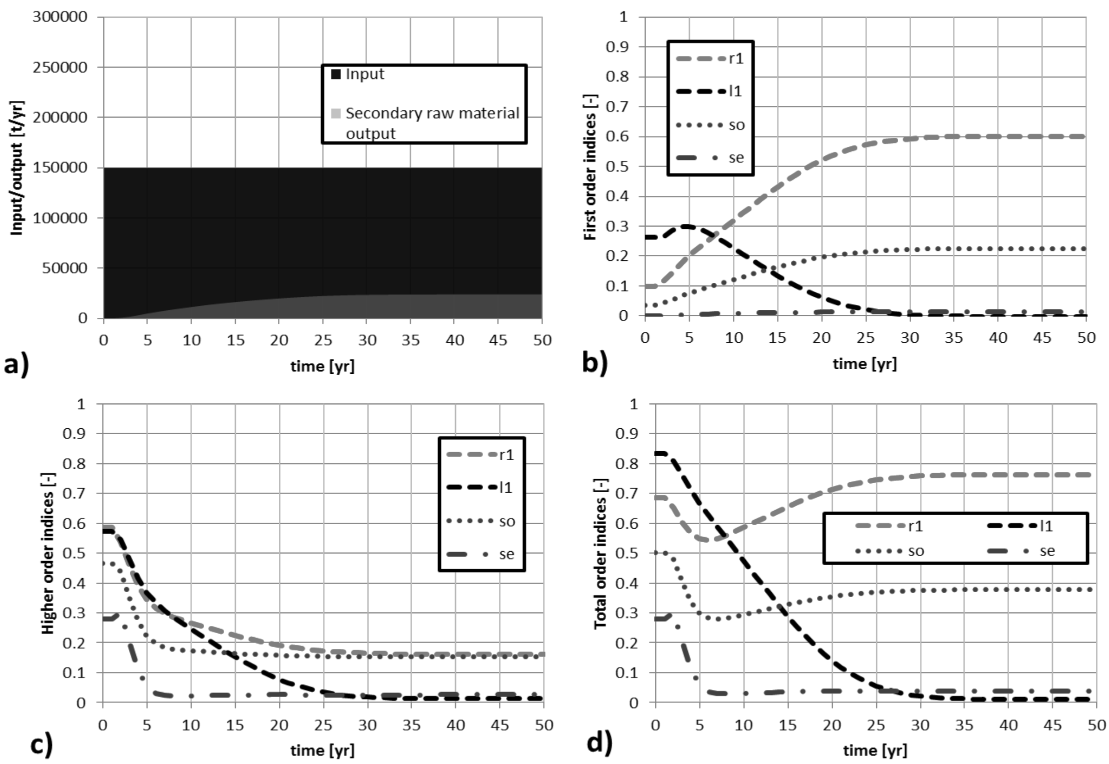

Figure S3: Sensitivity indices for a secondary raw material output: Illustration of (a) the input and output, (b) the first order, (c) higher order and (d) total order indices.

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Article III:
Evaluation of modeling approaches to determine end-of-life flows associated with buildings: a Viennese show case on wood and contaminants

Nađa Džubur and David Laner

Journal of Industrial Ecology, under revision.

Evaluation of modeling approaches to determine end-of-life flows associated with buildings: a Viennese show case on wood and contaminants

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Summary

Dynamic material flow analysis (MFA) enables forecasts of secondary raw material potentials of waste volumes in future periods by assessing past, present, and future stocks and flows of materials in the anthroposphere. Analyses of waste streams of buildings stocks are uncertain with respect to data and model structure. Wood constructions in Viennese buildings serve as a case study to compare different modeling approaches for determining end-of-life (EOL) wood and corresponding contaminant flows (lead, chlorine, and PAH). A delayed input and a leaching stock modeling approach are used to determine wood stocks and flows from 1950 until 2100. Cross-checking with independent estimates and sensitivity analyses are used to evaluate the results' plausibility. Under the given data situation in the present case study, the delay approach is a better choice for historical observations of EOL wood and for analyses at a substance level. It has some major drawbacks for future predictions at the goods level, though, as the durability of a large number of historical buildings with considerably higher wood content is not reflected in the model. The wood content parameter differs strongly for the building periods and has therefore the highest influence on the results. Based on this knowledge, general recommendations can be derived for analyses on waste flows of buildings at a goods and substance level.

Keywords

Building stock modeling, end-of-life wood, contaminants, dynamic MFA/SFA, uncertainty analysis

<heading level 1> Introduction

Dynamic material flow analysis (MFA) aims to quantify material flows and stocks over time. Historic development patterns of material stocks and flows are often used to create scenarios to estimate potentials of resources for the years and decades to come (Müller 2006). Using anthropogenic resources as secondary raw materials reduces the extraction of primary raw materials, which makes recycling a key strategy in promoting resource efficient economies (European Commission 2011). Apart from substituting primary raw materials, recycling is often beneficial also from an environmental perspective (Huang et al. 2015). Therefore, recycling has gained more and more popularity in the recent decades and there are various initiatives pointing out the potential value of secondary raw materials. Major waste streams, and thus potential secondary raw materials in urban areas, result from the demolition of buildings (Kleemann et al. 2016a). By now, waste generation from C&D (=construction & demolition and renovation) activities are major contributors to society's total waste flows and the magnitude of C&D waste is expected to further increase over the next few decades (Bergsdal et al. 2007). However, the longevity of buildings and thus the long residence time of their potential resources in stock may lead to an aggregation of contaminants in the stock, which may pose quality constraints for future recycling activities (Brunner 2010, Pivnenko et al., 2016).

The dynamics of building stocks, and therefore also the dynamics of aggregations of contaminants, are hard to analyze since data is scarce on the input side and is mostly a result of estimations, not only with regard to the substance but also with respect to the goods level (Kohler and Hassler, 2002). Thus, uncertainties arise not only at the goods level and at the substance level, but are also associated with the driving input parameters, such as the inflow to the use phase and the duration in use. Beside the uncertainty caused by the diversity of residential structures and building types as well as their material contents, lifetimes of buildings vary strongly and are therefore hard to determine. Furthermore, there are only a few material flow studies on stock dynamics on the goods together with the substance level by now. Studies on comparing structures of stock models at the substance level have been published by van der Voet et al. (2002) and Kleijn et al. (2000). Both studies compare a delay approach based on lifetime considerations of the input to a leaching approach based on a leaching share of the stock. While van der Voet et al. (2002) present analytical conditions under which the calculations of the leaching approach will produce acceptable solutions for dynamic models, which should typically be solved using the delay approach, Kleijn et al. (2000) show preliminary versions of the approaches using signal processing for the estimation of emissions. In the present article, we build on these two archetypal modeling approaches and extend them to more accurate models for EOL wood flows associated with buildings in Vienna.

In the delay approach, EOL wood flows and contaminants contained therein (lead, chlorine, and polycyclic aromatic hydrocarbons (PAH)) are determined based on past wood inputs and product lifetimes (i.e. residence time of wood constructions in use). In the leaching approach, bottom-up estimates of the wood stock in buildings at different times are combined with estimates of demolition and renovation rates to calculate the output of wood and contaminants from the use phase. These two modeling approaches are compared in the present study using the case of wood stocks and end-of-life wood flows of Viennese buildings. The goal is to investigate the data requirements of each approach and the effects of inherent modeling assumptions on the resulting stocks and flows of wood and the contaminants contained therein (Pb, Cl, PAH).

The article is organized as follows: In Section 2, a categorized literature review of dynamic MFA studies modeling construction and demolition waste of buildings is presented. In section 3, the case study, which is analysed from both a historical perspective and a projected demand scenario, is presented at the goods and substance level. The section contains the uncertainty assessment of the underlying data, the treatment of uncertainty, the description of the modeling approaches, the investigation of the cross-checking of the results and, finally, sensitivity analysis with regard to its critical factors. The calculation results are presented and explained in section 4. Section 5 contains a discussion of the results and highlights major findings regarding the explanatory power of each approach and the recommendations which can be derived from the comparison of the approaches. Conclusions are presented in section 6.

<heading level 1> Building waste in dynamic MFA

Various dynamic MFA studies on C&D waste of the building sector have been published in the past decade. Dynamic MFA studies are differentiated between top-down studies (mass balance-driven, derivation of stock out of time series) and bottom-up studies (consist of summing up the amount of material contained in all relevant products in the various sectors, see Laner & Rechberger, 2016). The modeling approaches used in bottom-up studies are based on accounting. The methods used in top-down studies are further differentiated in input-driven (driven by the input in the stock) and stock-driven (driven by service units provided by the in-use stock) approaches (cf. Müller et al. 2014). Furthermore, the modeling approach can either be a delay approach (based on lifetime functions) or a leaching approach (based on fractions of the presented stock, see van der Voet et al. 2010).
A bottom-up study was presented by Lichtensteiger and Baccini in 2008 by combining architectural know-how and geoscience approaches to explore stocks of buildings and material contents. In 2015, Tanikawa et al. published a bottom-up study by mapping the building material stock of Japan in great detail, including the incorporation of the know-how of previous studies. In contrast to the study by Tanikawa et al., we use the term "top-down" related to the method of determining the stock, which designates the distinction of sectors in the stock and is characterized by splitting the total input into different sector inputs.

Most top-down studies which focus on the building sector rather than on specific goods (where the building sector is included) are driven by stocks and calibrated with existing data since continuous time series data are hardly available and hard to estimate. Consequently, an input-driven approach is highly uncertain. A model on the analysis of waste wood streams from buildings was published by Müller et al. (2004) focusing on timber management in general. In the paper of Müller et al. (2006), the focus was on the dynamics of the building stock of the Netherlands. In that paper, they analyzed and calibrated the stock with regard to the major drivers, such as population, lifestyle (floor area per person) and material intensity. The aim was to give a future prognosis by observing scenarios. Bergsdal et al. (2007), Sartori et al. (2008), Brattebo et al. (2009), and Sandberg et al. (2014) adapted this model to analyze the behavior of Norway's dwelling stock (cf. also Augiseau et al. 2016). Based on the same idea, Pauliuk et al. (2013) proposed a model with an optimization routine to identify buildings with the highest saving potentials. Also Hu et al. (2010a) adapted this generic model to analyze the building stock of Beijing. In Hu et al. 2010b, the model was used for China and extended to incorporate reflection on urban and rural relationships. Also Huang et al. (2012) modelled the dynamic building stock of China based on this generic model. Miatto et al. (2017) presented a comparison of lifespan assumptions for different input-driven top-down case studies.

The studies mentioned used a delay approach by considering the specific lifetimes of dwellings. Schneider and Rubli (2007) adapted a leaching approach to a dynamic MFA study on the building stock of Zürich. Together with a detailed MFA, scenario analysis of changes of the building stock and input and output flows over time are presented depending on exogenous factors. Gallardo et al. (2014) used the leaching approach presented by Kleijn et al. (2000) to implement a dynamic model of the building stock of Chile to observe the vulnerability of the building stock to earthquakes. A categorization of all those studies with regard to the main modeling assumptions can be found in Table 1.

Table 1: Literature on dynamic MFA studies of C&D waste

Authors	City/State, time span	Method	Modeling approach	Focus
Müller et al. (2004)	Swiss lowland region, 1900-2100	Top-down, stock-driven	Delay	Analysis of wood and energy flows of the timber management, including building waste wood; calibrated until 1997 and continued using scenarios
Müller et al. (2006)	The Netherlands, 1900-2100	Top-down, stock-driven	Delay	Analysis of stock dynamic behavior of C&D waste based on scenarios
Bergsdal et al. (2007)	Norway, 1900-2100	top-down, stock-driven	Delay	Analysis of stock dynamic behavior of the environmental metabolism, including scenario analysis based on the generic model by Müller et al. 2006
Sartori et al. (2008)	Norway, 1900-2100	top-down, stock-driven	Delay	Analysis of renovation activities for energy savings based on the model by Müller et al. 2006; scenarios and comparisons to test input uncertainties
Brattebo et al. (2009)	Norway, 1900-2100	top-down, stock-driven	Delay	Generic model based on Müller et al., 2006, is used for quantification of the material and energy metabolism and its corresponding economic and environmental suitability for analyzing building and road bridge stocks
Sandberg et al. (2014)	Norway, 1900-2050	top-down, stock-driven	Delay	Model, based on Müller et al. 2006, is used to give insights into what segments of the dwelling stock that are expected to be exposed to renovation in the future.
Pauliuk et al. (2013)	Norway, 2010-2060	Top-down, stock-driven	Delay	Novel dynamic stock model with optimization routine to identify and prioritize buildings with the highest saving potentials
Hu et al. (2010a)	Bejing (China), 1900-2100	Top-down, stock-driven	Delay	Recommendations on C&D waste management based on scenarios of the generic model by Müller et al. 2006
Hu et al. (2010b)	China, 1900-2100	Top-down, stock- driven	Delay	Analysis of the stock dynamic behavior and scenario analysis based on the generic model by Müller et al. 2006, extended with reflections on urban and rural relationships

Huang et al. (2012)	China, 1950-2050	Top-down, stock-driven	Delay	Estimations of the long-term material demand and environmental impacts
Miatto et al. (2017)	Japan, US, UK, 1950-2000	Top-down, input-driven	Delay	Investigation into lifetime distributions and uncertainties about stock accumulations, comparisons for three cities
Gallardo et al. (2014)	Chile, 1950-2100	Top-down, stock-driven	Leaching	Dynamic modeling of the building stock using a quantitative assessment method to observe the vulnerability of the building stock to earthquakes
Tanikawa et al. (2015)	Japan, 1945-2010	Bottom-up	Approach based on accounting	Review of the state of art of material stock research and presentation of a project on mapping construction material stocks
Lichtensteiger & Baccini (2008)	Switzerland, 1900-2000	Bottom-up	Approach based on accounting	MFA in combination with architectural know how and approaches inspired by geosciences are used to explore urban stocks in buildings, the combination of material contents, and scenario analyses to explore future trends
Schneider & Rubli (2007)	Zürich (Switzerland), 1995-2050	Top-down, stock-driven	Leaching	MFA and scenario analysis of changes in the building stock and in input and output flows over time depending on exogenous factors

<heading level 1> Material and Methods

<heading level 2> Case study on EOL wood flows from buildings in Vienna at the material and substance level

The proposed case study for the dynamic MFA material flow model examines the wood stock in Viennese buildings together with its demolition activities that has been investigated in a GIS-based analysis by Kleemann et al. (2016b). The variables of interest are, on the one hand, the amount of EOL wood flows resulting from the demolition and renovation of buildings, including beams in wood (roofs, ceilings) and wood extension products (windows, doors, floors and others). On the other hand, the substance level is considered with regard to the quality of wood flows in terms of contaminants and impurities (lead, chlorine, PAH). These contaminants are chosen as they have been observed at elevated levels in waste wood collected for recycling, i.e. directed towards particle board production (BMLFUW, 2012). The sources of the contaminants are wood preservatives which were used in the past (and are nowadays forbidden), on the one hand, and coatings and adhering particles, on the other. As the amount of wood in buildings is strongly correlated to the construction period (Kleemann et al. 2016b), the amounts of wood as model input parameters are classified according to the construction period of the respective building. Moreover, as all contaminants have been used in applications that were forbidden in the course of time, the substance flow variables depend on time. The model is used to estimate the amount of EOL wood flows, and lead, chlorine and PAH in EOL wood flows from demolition and renovation activities in Vienna over time employing all available information on the flows and stocks of wood in the building sector.

<heading level 2> Data and uncertainty analysis

The following section presents the data used to estimate the flows of EOL wood and of the selected substances. A classification of the data with respect to its uncertainty can be found in Table 2. The measurement unit of the input data and the results are metric tonnes. Uncertainty levels are assigned to the data based on the method suggested by Hedbrant and Sörme (2001). In this study, 4 levels of uncertainty are differentiated, whereby level 1 represents national stastistics or independent research studies, with level 4 indicating rough estimates ((see also Laner et al 2015 (uncertainty concepts) and Dzubur et al. 2016 (uncertainty characterization)). The data is fed into the model, all variables of which are assumed to be normally distributed. Standard deviations for the densitiy functions are derived from results obtained from the underlying uncertainty function. Level 1 has a standard deviation of 4.5%; for level 2, it is 9.9%, for level 3, 22%, and for level 4 it is 49.1%.

Table 2: Classification of data (Abbreviations: UL… uncertainty level)

<table>
<tr><th>Type of data</th><th>Amount of data (year/period)</th><th>Source</th><th>UL</th></tr>
<tr><td>1.Building stock of Vienna</td><td>
<table>
<tr><td>Year</td><td>Number of buildings</td></tr>
<tr><td>1951</td><td>72948</td></tr>
<tr><td>1961</td><td>79034</td></tr>
<tr><td>1971</td><td>96209</td></tr>
<tr><td>1981</td><td>134321</td></tr>
<tr><td>1991</td><td>153693</td></tr>
<tr><td>2001</td><td>168167</td></tr>
<tr><td>2011</td><td>164746</td></tr>
</table>
</td><td>National Statistics Austria, 2011</td><td>1</td></tr>
<tr><td>2.Categorization of age classes of building stock of Vienna</td><td>
<table>
<tr><td>Share of age class/year</td><td>-1918</td><td>1919-1945</td><td>1946-1976</td><td>1977-1997</td><td>1998-</td></tr>
<tr><td>1950-1959</td><td>0.79</td><td>0.16</td><td>0.05</td><td>0.00</td><td>0.00</td></tr>
<tr><td>1960-1969</td><td>0.71</td><td>0.15</td><td>0.14</td><td>0.00</td><td>0.00</td></tr>
<tr><td>1970-1979</td><td>0.58</td><td>0.12</td><td>0.27</td><td>0.00</td><td>0.00</td></tr>
<tr><td>1980-1989</td><td>0.42</td><td>0.09</td><td>0.30</td><td>0.20</td><td>0.00</td></tr>
<tr><td>1990-1999</td><td>0.37</td><td>0.08</td><td>0.26</td><td>0.30</td><td>0.00</td></tr>
<tr><td>2000-2009</td><td>0.33</td><td>0.07</td><td>0.24</td><td>0.27</td><td>0.09</td></tr>
<tr><td>2010-2020</td><td>0.34</td><td>0.07</td><td>0.24</td><td>0.25</td><td>0.12</td></tr>
</table>
</td><td>Kleemann et al. 2016b (2010-2020)
Rough Estimates (1950-2010)</td><td>4</td></tr>
<tr><td>3.Wood contents for age classes (tonnes) per building for each construction period</td><td>
<table>
<tr><td>Period</td><td>Tonnes/ building</td></tr>
<tr><td>-1918</td><td>99.6</td></tr>
<tr><td>1919-1945</td><td>35.1</td></tr>
<tr><td>1946-1976</td><td>24.5</td></tr>
<tr><td>1977-1996</td><td>18.2</td></tr>
<tr><td>1997-</td><td>12.7</td></tr>
</table>
</td><td>Kleemann et al. 2016b</td><td>2</td></tr>
<tr><td>4.Shares of wood products in buildings of different time periods</td><td>
<table>
<tr><td>Share</td><td>-1918</td><td>1919-1945</td><td>1946-1976</td><td>1977-1997</td></tr>
<tr><td>Windows</td><td>0.067</td><td>0</td><td>0.1</td><td>0</td></tr>
<tr><td>Doors</td><td>0.04</td><td>0</td><td>0.17</td><td>0.06</td></tr>
<tr><td>Roofs</td><td>0.5</td><td>0.695</td><td>0.11</td><td>0</td></tr>
<tr><td>Floors</td><td>0.013</td><td>0.07</td><td>0.22</td><td>0.92</td></tr>
<tr><td>Ceilings</td><td>0.31</td><td>0.007</td><td>0</td><td>0.02</td></tr>
<tr><td>Other wood products</td><td>0.03</td><td>0.043</td><td>0.367</td><td>0</td></tr>
</table>
</td><td>Kleemann et al. 2016b</td><td>3</td></tr>
<tr><td>5.Lead, chlorine and PAH values for each wood product (same as above)</td><td>
<table>
<tr><td>Amount (mg/tonnes wood)</td><td>Lead</td><td>Chlorine</td><td>PAH</td></tr>
<tr><td>Windows</td><td>29390100</td><td>550000</td><td>35800</td></tr>
<tr><td>Doors</td><td>2676700</td><td>620000</td><td>15300</td></tr>
<tr><td>Roofs</td><td>19100</td><td>329800</td><td>2000</td></tr>
<tr><td>Floors</td><td>1300</td><td>495000</td><td>33200</td></tr>
<tr><td>Ceilings</td><td>1600</td><td>5121000</td><td>300</td></tr>
<tr><td>Other wood products</td><td>389300</td><td>622200</td><td>2300</td></tr>
</table>
</td><td>Environmental Institute of Vorarlberg 1999;
BUWAL Switzerland 2004</td><td>3</td></tr>
<tr><td>6.Demolition rate</td><td>0.3%
(value for 2013; assumed to be constant over time)</td><td>Kleemann et al. 2016b
Stäubli et al. 2010</td><td>2</td></tr>
<tr><td>7.Renovation rate</td><td>1.1% (2009-2012 ; assumed to be constant over time)</td><td>IIBW 2012</td><td>2</td></tr>
<tr><td>8.Technical lifetimes of wood</td><td>
<table>
<tr><td>Product</td><td>Lifetime (in years)</td></tr>
<tr><td>Windows</td><td>50</td></tr>
</table>
</td><td>SwissBauCo 2009;
IIEMB 2006;
Reis 2012</td><td>2.5</td></tr>
</table>

products in buildings	Doors	50		
	Roofs	120		
	Floors	50		
	Ceilings	60		
	Other wood products	40		

<heading level 2> Treatment of Uncertainty

In a first step, normal distributions with mean values according to the respective sources and standard deviations according to their uncertainty level are assigned to the various input data (see Table2). The building stock is multiplied with the content of wood according to the age class of the building and divided into the 6 types of wood categories in a next step. The categorization of the building stock needs to be considered for the leaching approach. In order to get the shares of the wood of buildings resulting as a product of these variables (data type 1.-4. in Table 2), an approximation of the product of the normally distributed probability density functions is used. As the product of normally distributed functions is not normally distributed, we consider a normally distributed approximation where the mean of the product of $N(\mu_1, {\sigma_1}^2), N(\mu_2, {\sigma_2}^2)$ is the product of the means $\mu_1\mu_2$ of the normally distributed variables μ_1, μ_2 and the standard deviation is approximately $\sqrt{\sigma_1^2\sigma_2^2 + \mu_1^2\sigma_2^2 + \mu_2^2\sigma_1^2}$ (Ware & Lad, 2003). In the leaching stock approach, mulitplications are done with the densitiy functions of the demolition and renovation rate (following a cyclical pattern, see next section), for which the densitiy functions are summed up at first. Monte Carlo simulation runs are performed on these final shares. Furthermore, lead, chlorine and PAH values per wood product category (6. in Table 2) are assumed to be normally distributed and Monte Carlo simulation runs are performed on them. In the delay model, the technical lifetimes for the building wood products are calculated in an analagous manner to that of the Monte Carlo simulation.

<heading level 2> Modeling Approaches & Assumptions

It should be emphasized that stylized models of wood stocks and flows associated with Viennese buildings are used to investigate the effect of differences in the modeling approaches on the outputs rather than to give a highly realistic picture of the Viennese situation. For the latter, more elaborate data mining and additional information on key input parameters (e.g. specific lifetime functions, analysis of the variation of demolition and renovation rates over time for Vienna, etc.) would be required. However, this is outside the scope of the present study.

Because demolitions of buildings are mainly carried out when they are planned to be replaced by new buildings, and as both demolitions and renovations of buildings are cost-intensive, it is assumed that the actual output of EOL wood is externally influenced by the business cycle. Thus, the higher the turnover of the building industry, the more there is to be demolished and renovated, with the rest remaining in a pool of “depleted buildings” of the stock, which represents a hibernating stock in both models. While the leaching approach reflects the current economic situation (provided real-time data is available), meaning that the business cycle has a direct influence on the rate of renovations and demolitions in a specific year, the delay approach is lifetime-based, meaning that only a very small percentage of buildings at the end of their lifetimes is assumed to depend on the business cycle (in order to enable extensions of lifetimes). The amplitude of the business cycle and its approximate behaviour are based on the investment in construction activities data from the Austrian Institute of Economic Research (WIFO Economic Data Service, 2016). All formulas used for the modelling approaches and assumptions are presented in SI-1 of the Supporting Information (=SI).

Because PAH and lead coatings were banned in the middle of the 90s (ChemG, 1996; see RIS, 2016) and chlorine components have been increasingly replaced since then, it is assumed that input from demolition wood of wood products from the middle of the 90s (1998-) on is free of those contaminants.

In order to extend the models to predict the future development of building EOL wood flows and contaminants from 2020 on, the building stock is assumed to rise by 0.38% annually, starting with the initial stock value in 2011. This assumption is based on the prediction of a growing Viennese population (Statistik Austria, 2014a) and the average number of buildings per 1000 inhabitants (Statistik, Austria, 2014b), assuming a constant per capita floor area (cf. also Statistik Austria, 2014b).

<heading level 3> Leaching stock approach

The data of the building stock is given for the first year of each decade. Every stock is classified into age categories. The demoliton rate and the renovation rate are summed up. This sum is assumed to be constant over time. The behaviour of the business cycle is assumed to be cyclical with a period of 20 years. The output O (in tonnes of wood) is then calculated as a leaching part of the stock for each year t, thus,

$$O(t) = f(t, c + r) * S(t), \qquad \text{Equation (1)}$$

whereby f is the sine function of the business cycle which depends on the mean value c+r of the stock, c is the demolition and r the renovation rate, and S the stock of building wood (for more detailed information see also SI-1 a),c)).

<heading level 3> Delayed input approach

This model builds on the knowledge of newly built buildings within each decade since 1950. There is no data provided for this input. The change in stock is the net growth of the number of buildings in Vienna. The input is the sum of the net growth and the overall output of each building period, which is determined by means of the age categories of the stock in each period (the difference of buildings in stock of each age category between two decades, see SI -1 b)). Due to a lack of higher temporal resolution, the changes are split equally over each period of 10 years. The evolution of the initial stock (built up before 1950) is estimated with the aid of the classification of age categories of the stock. This initial stock is split into buildings from the past up to 1918 and buildings from 1919-1945. The amount of wood in the stock is determined based on the wood content of each product category in each construction period. The products within a period are assigned the associated technical lifetimes. The output O_i of waste wood of each product category i (i=1,..,6) is calculated as a delayed share of input in each year t, which depends partly on the business cycle (with a share of (1-p)). As the major part of Vienna's building stock is inhabited or in use, there is a high turnover of constructions and renovations and therefore, a need for replacement at the end of the technical lifetimes. Thus, the variable p, which represents the share which is not influenced by the buisness cycle, is assumed to be 99%. The output of a construction product category is

$$O_i(t) = pI_i(t - L_i) + f(t, 1 - p)I_i(t - L_i), \qquad \text{Equation (2)}$$

whereby f is the same sine function as in the leaching approach with a mean value of 1-p=1%, I_i is the amount of wood of product i going into the stock, and L_i is the product lifetime following a Weibull distribution (with a normally distributed mean value). The overall output is

$$O(t) = \sum_{i=1}^{6} O_i(t) \qquad \text{Equation (3)}$$

for each year (see also SI-1 b),c)).

The comparison of the approaches is not only done on output flows but also on the stocks in order to analyze the differences in amounts and therefore, the differences within the approaches in full. The substance level is calculated by mulitplying the wood products with the respective substance concentrations in both approaches (cf. SI-1).

<heading level 2> Cross-checking of model results

The results of the modeling approaches are cross-checked with independent estimates in order to get an impression on how well the model outputs fit the data values. The amount of waste wood is estimated to be 64,650 tonnes in 2013, which is the per-capita share for Vienna (UN data, 2013) of the total amount of demolition wood in Austria (BMLFUW, 2013). The uncertainty level of this cross-checking value is 2, thus, the standard deviation is 9.9%. On the substance level, representative contents of lead, chlorine and PAH are derived from a study on waste wood flows in Switzerland (Buwal,2004). These estimates are quite uncertain as the samples taken vary strongly for each wood product category. The substance concentrations, given by mean and standard deviation, are then multiplied with the amount of waste wood in Vienna to determine the substance flows in the year 2013. This results in an estimated amount of PAH in Viennese waste wood of 1.1 tonnes per year with a standard deviation of approximately 20% of the mean value (numerical approximation, see Treatment of Uncertainty). The amount for lead is 31.6 tonnes/yr, varying with a standard deviation of 205% (with the minimal value of 0) and the amount of chlorine is 49.9 tonnes/yr with a standard deviation of 204.5% of the mean (again, restricted to positive values).

<heading level 2> Sensitivity Analysis of model parameters

Sensitivity analysis is used for the identification of critical parameters, whose variation has the largest effect on the variation of the model results. This increases the understanding of the relationships between input and output variables of a model. The model outputs are analyzed for a) the impact of specific parameter perturbation (local sensitivity analysis) and b) the overall distribution of the uncertainty of the output (global sensitivity analysis, cf. Dzubur et al. 2016).

<heading level 3> Local sensitivity analysis of the input parameters

While demolition and renovation rates are critical parameters in the leaching approach, the lifetimes are the respective counterparts in the delay approach. Both are tested for minor and major perturbations.

As the share of initial stock up to 1918 has the far highest wood content and therefore plays a major role in both modeling approaches, and as its actual magnitude is highly uncertain, scenarios are tested for the reallocation of amounts of this building stock to later building periods. The results are analyzed for the EOL wood flows.

The effects of shares of specific building periods are tested for their influence on the EOL substance flows of PAH in order to find out which period influences recent outputs (with a focus on 2010) the most.

<heading level 3> Global sensitivity analysis of the overall systems of EOL wood and contaminants

In a first step, all parameters are tested for their first order effects (effects without interactions with other parameters) on the model output (EOL wood flows, substance flows) using the EASI algorithm (cf. Plischke et al. 2010). In a next step, the output flows (at the goods level) are also analyzed for bundled groups of parameters as input parameters, the shares of wood categories, which enter the stock in each year. Detailed information can be found in SI-3 in the SI.

<heading level 1> Results

<heading level 2> Comparison of EOL wood flows and stocks

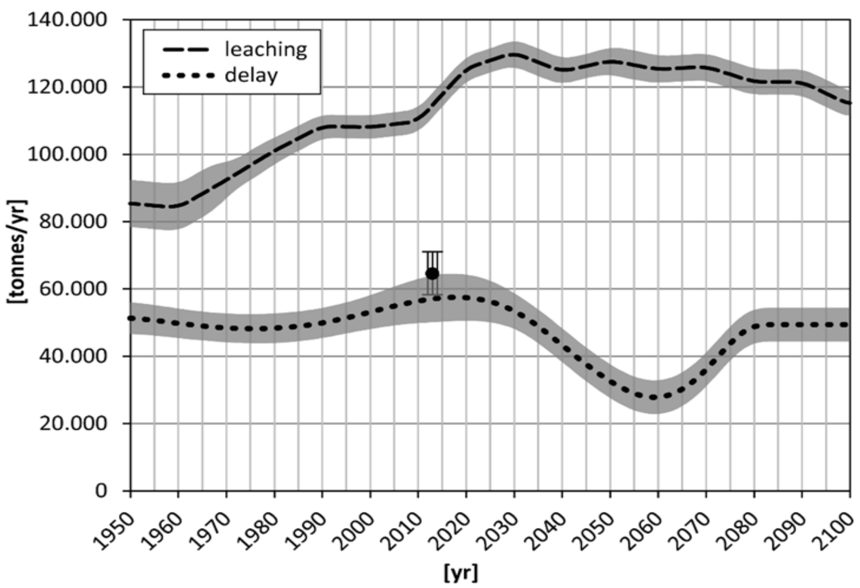

Fig 1: Flows of EOL wood from demolition and renovation activities for leaching and delay approach (mean values indicated by black lines, range of ± one standard deviation indicated by grey shaded area) and cross-checked with data from 2013 (black dot) and its standard deviation in the whiskers.

In Figure 1, a comparison of EOL wood flows (from demolition and renovation) between the leaching and the delay approach is shown. The results are shown as mean values (black lines) together with the range of one standard deviation (i.e. 68% of the model results are contained in this range).

The delay model reaches its peak around 2020. This peak is mainly caused by the dominating number of roofs up to 1918 but also by the large number of floors from 1977-1997. Compared to these amounts of wood, the rest is of secondary importance. Although the number of houses in Vienna is rising, the share of wood in houses is remarkably lower from the end of the 20th century on than it was in the beginning of that century (see Table 2, 3.). The peaks in the outputs of the delay and leaching approach are shifted. The reason is the large number of roofs up to 1918, leaving the stock about 120 years later in the delay approach. In contrast to that, the output in the leaching approach is rather driven by the size of the historical building stock. Although the number of buildings is rising in the future prognosis, the amount of EOL wood is slightly shrinking in total as the number of buildings with high wood-concentrations is shrinking in the stock.

While the influence of the business cycle can slightly be seen in the fluctuations of the leaching approach in the future prognosis, these fluctuations are not observable in the delay model. The reason for the minor importance of the business cycle in the delay approach is that only 1% of buildings at the end-of-life are affected by the business cycle, whereas the remaining 99% generate output as defined by the lifetime functions.

From Figure 1 it is apparent that the cross-checking value for waste wood lies between both model approaches but only the range of the flow of the delay approach is within the standard deviation. Whereas the mean of the EOL output of the delay approach is relatively close, the EOL wood flows of the leaching approach are far above this value.

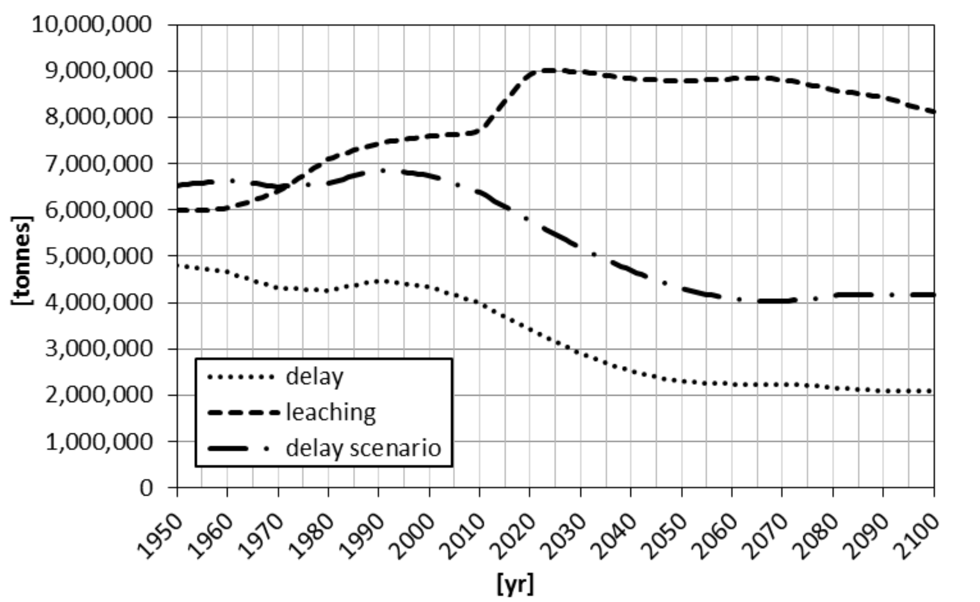

Figure 2: Comparison of wood in stock (only mean values shown) for the leaching approach, delay approach and a scenario with changes in the initial stock of the delay approach

A comparison of the stock size of building wood is given in Figure 2 (for the mean values of the results). It can be seen that in the leaching approach, not only are the ouput flows far higher than in the delay approach (cf. Figure 1), but the stock size is also more than 1,000,000 tonnes higher at the beginning of the modeling period and more than double the amount at the end. A major reason is that the technical lifetimes may be too short with regard to the initial stock (up to 1918, 1919-46). Very old wood components tend to be of better quality as they are made of solid wood in general, in contrast to present wood components, which mostly contain wood composites.Therefore, a scenario with doubled lifetimes for the initial stock is tested for the delay approach. It can be seen that this scenario leads to a larger stock size (for about 500,000 tonnes) than the leaching approach at the beginning period of observation, but also falls below the leaching approach thoughout the modeling period as the lifetimes of the subsequent buildings in stock are shorter than those of the initial stock.

<heading level 2> Comparison of substance flows

The contaminants lead, chlorine and PAH don't appear, or respectively, are replaced in wood products after 1996. Thus, the last input of substances is given in the 90s decade in the delay approach, and the last share of age class with contaminant input considered in the leaching approach is 1977-1997. In Figure 3, the comparison of lead in EOL wood flows (means and ranges) is shown for the two approaches. The comparison of chlorine is shown in Figure 4 and the comparison of PAH in Figure 5. All substance flows show a similar behavior to the flow at the goods level in the leaching approach. This is due to the fact that the shares of the products over a period are aggregated. Each output flow consists of a part of each period of input so that the flow of lead is balanced and not concentrated for a specific year or product, and thus it depends mostly on the input of goods. As there is no input on the substance level after 1996, the flows decrease faster than the EOL wood flows. However, non-negligible values can still be found even after one century in the leaching approach. The substance flows in the delay approach show slightly shifted peaks compared to the EOL wood flows. Furthermore, the substance flows decrease drastically after 2020 and are negligible from 2050 on according to this approach.

The highest amount of lead and chlorine can be found in wood from the period up to 1918(lead from windows and chlorine from ceilings), leading to high amounts at the beginning of the flow observations for both approaches. The share of this period shrinks slightly in the leaching approach for both substance flows. There is almost no PAH in buildings up to 1918, which is reflected in the results of both approaches.

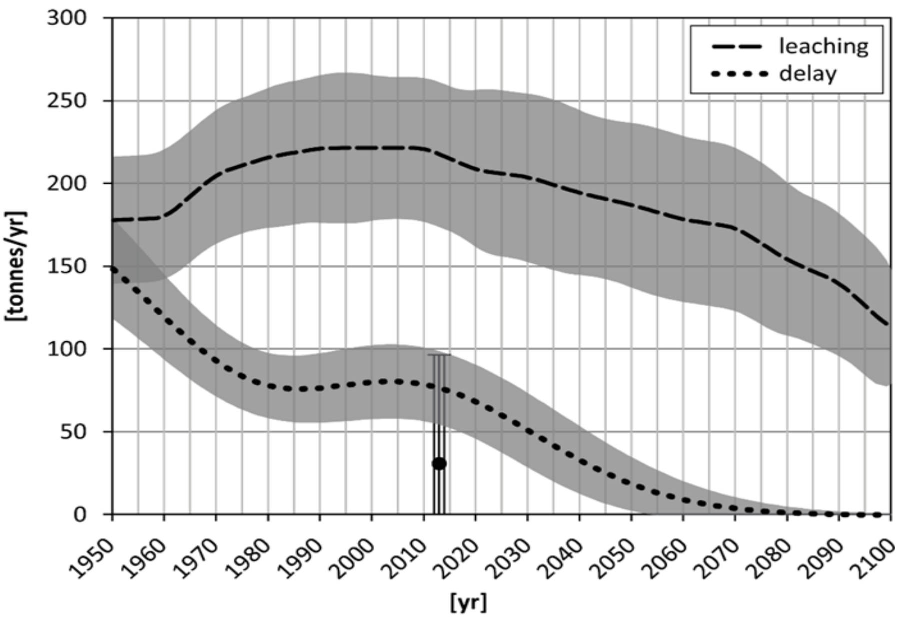

Fig 3: Lead flows in EOL wood (mean values and standard deviation ranges) and data cross-check for lead in waste wood, including standard deviation (in the whiskers)

The lead flow reaches another slight peak in the delay approach resulting again from the high concentration of lead and the high share of windows input in the period 1946-1976 (see Figure 3). Windows have the highest amount of lead since lead was used for plastic coatings and color pigments. The comparison with the cross-checking data value shows that the mean values of both models substantially overestimate the mean value (factor 2.5 to 7.5). However, due to the high uncertainty of the independent estimate for lead in EOL wood, the range of the lead flow calculated by the delay model (including 68% of the results) lies within the standard deviation's range.

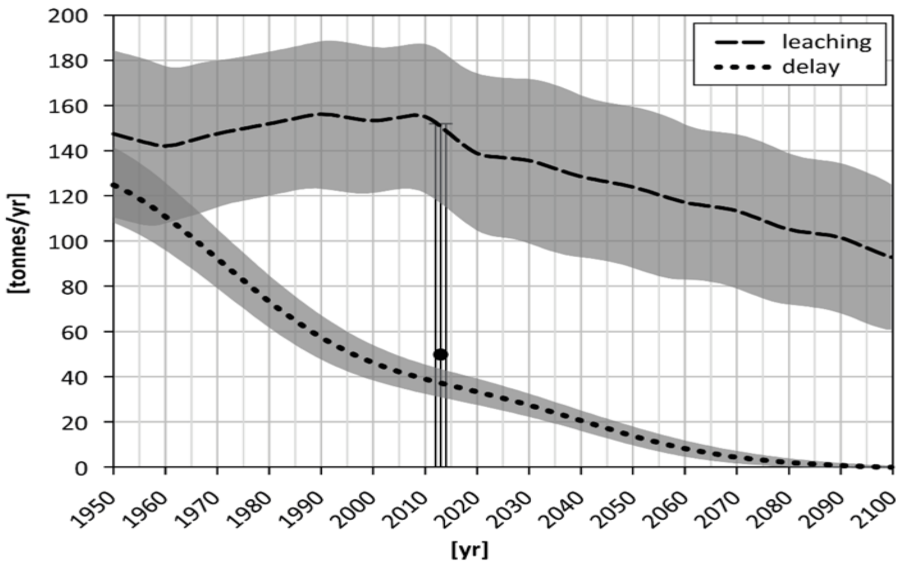

Fig 4: Chlorine flows in EOL wood (means and ranges) and data cross-check for lead in waste wood (black dot), including standard deviation (designated by the whiskers)

Ceilings and roofs from 1919-1945 have a slight impact on the chlorine flows observable in the delay approach (see Figure 4). Chlorine was used as a hardener component in glue that was used for beams in wood. The cross-checking value of the average chlorine amount lies between both models, and is close to the result of the delay model.

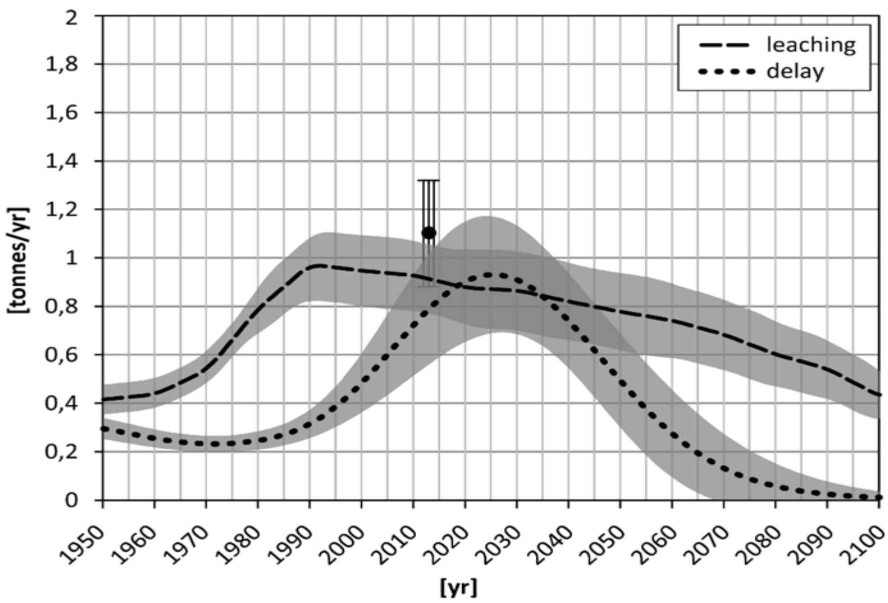

Fig 5: PAH flows in EOL wood (mean values and standard deviation ranges) and data cross-check for lead in waste wood (black dot), including standard deviation (designated by the whiskers)

The growth of the PAH flow at the end of the 20^{st} century in the leaching approach is caused by the rising number of floors from 1919 on reaching their end of life (see Figure 5). PAH from creosote was often used to attach parquet, but also as a preservative on windows. In the delay approach, the highest PAH flow value is mainly caused by the high number of floors from 1977-1997, and the high number of floors and windows from 1945-1977, which are all aggregated in the output flow between

2020 and 2030. The amounts of PAH in other wood products are negligible. The cross-checking mean value for PAH is slightly underestimated by both approaches. However, the ranges of both approaches lie within the standard deviation of the cross-checking value.

<heading level 2> Results of sensitivity analysis

<heading level 3>Local sensitivity analysis of the input parameters

Perturbations on the lifetimes in the delay approach and demolition and renovation rates in the leaching approach behave linearly with regard to the EOL output flows (see Figure SI-2.1 a) and b) in the SI). Thus, in the delay approach, an increase in lifetimes goes hand in hand with an increase in the material stock as well as a decrease in output flows (at least as long as the stock is still growing). Outputs from the leaching approach change directly proportional to changes in demolition and renovation rates.

The effect of considering fewer buildings from the period up to 1918 and therefore, more from all other periods, is tested at the goods level. In both approaches, the reallocation of buildings into periods after 1918 leads to a drastic decrease of EOL wood flows (see Figure SI-2.2 a) and b) in the SI).

Historical effects of substance applications on current periods are tested on the example of PAH for the year 2010 (see Figure SI-2.3 a) and b) in the SI). It can be seen that PAH aggregations from the initial periods (up to 1918 and 1919-1945) have the highest effect on the PAH output flow in the leaching approach, followed by the effects from 1977-1997. For the delay approach, the amount of PAH from 1977-1997 has the highest effect by far, while the amounts of PAH from the initial stock are negligible. This result is more reliable because for the leaching approach, the consideration that buildings from the period up to 1918 and 1919-1945 are renovated with PAH-free wood is ignored, leading to an overestimation of PAH values from these periods.

<heading level 3> Global sensitivity analysis

By testing the EOL wood flows at the goods level using the EASI algorithm, it can be observed that all first order effects make up less than 10% for both modeling approaches, meaning that the uncertainty of the output is mostly determined by interactions of the parameters. Therefore, the uncertainty of the main effects of the bundled shares of wood constructions is analyzed. In a next step, the substance level of contaminants from EOL wood is considered. The detailed results and further information can be found in SI-3 in the SI.

In the leaching approach, EOL wood flows are mainly sensitive to the share of roofs followed by ceilings in buildings from the period up to 1918. Because the wood content of modern buildings is relatively low and mainly constituted by floors, the share of floors becomes the most important model parameter during later model periods (after the end of the 20^{th} century). The EOL wood flows in the delay approach have similar sensitivities. Ceilings up to 1918 make up the most sensitive parameter until 1990, when roofs from the same period become the most important parameter. The sensitivity impact of the share of floors on EOL flows rises within the same time period as in the leaching approach by the end of the 20^{th} century.

PAH flows are mainly sensitive to the floor parameters in both approaches from 1980 on as floors are not only the main constructions in modern buildings but also have very high concentrations of PAH. The small share of windows up to 1918 also has high concentrations of PAH. The PAH flow until 1980 is sensitive to this share in the leaching approach while this share is already irrelevant in the period of observation in the delay approach.

Chlorine flows are mainly sensitive to the share of ceilings in both approaches as the concentration of chlorine in ceilings is tenfold higher than for all other wood constructions and as the share of ceilings up to 1918 is high.

As for the lead flows, the concentration of lead in windows is tenfold higher than for every other wood construction, and the share of windows is the most sensitive parameter for the lead flows in both approaches.

<heading level 1> Discussion

<heading level 2> Analysis of EOL wood flows on goods and substance level

The largest flow of EOL wood is related to the roofs and ceilings from buildings up to 1918. From a future perspective, we see that the amounts of waste wood will decrease although the number of buildings is on the rise. This is because of the low share of wood in modern Viennese buildings; mostly only floors are made of wood nowadays. This means that the peak in wood amounts which can be used as secondary resources is rather in the current period and won't play such an important role in the future.

More pronounced downward trends can be observed for the substance flows due to bans and replacements from 1996 on. However, although the peaks have already been reached, the amounts of contaminants deplete slowly. Consequently, lead, chlorine and PAH are expected to still be present in low levels in EOL wood over the next 50 years.

<heading level 2> Comparison of modeling approaches

<heading level 3>EOL wood flows

Leaching approach:

On the data level, poor information about the categorization of the building stock into different time periods causes a lot of uncertainty. However, this is not the main contributor to the big difference to the cross-check value. The uncertainty factor of the demolition and renovation rate is low. A major drawback of the approach is that the demolition and renovation rate are always taken with regard to the whole aggregated stock to calculate the output flows, ignoring the age of the buildings, and leading to highly overestimated amounts of waste wood (cf. also results on structure of stock in van der Voet et al. 2002). However, this drawback is of little importance for the future estimations of the amount of EOL wood under the scenario assumption that buildings in future periods will have the same wood content as nowadays.

Delay approach:

The input of buildings per period is unknown. It is calculated through the sum of change in stock each decade and the difference between buildings of each building period per decade. As already mentioned for the leaching approach, the categorization shares in building periods are uncertain parameters. Together with the fact that technical lifetimes are not always representative for the demolition/renovation of buildings (particularly, for the initial stock of buildings), this approach is very uncertain from a fitting of model and data perspective under the given circumstances. Lifetimes of buildings up to 1918 are supposedly too short, which has a particularly pronounced effect on the wood stock estimates (cf. delay scenario in Figure 2). However, with respect to EOL wood flows, the delay approach appears to result in more plausible estimates (cf. cross-check with waste wood in 2013 in Figure 1). The highest share of waste wood in Vienna originates from buildings up to 1918, which will be renovated with the same amounts of wood and which will remain stock. A shortcoming of the delay approach is that this is not accounted for, which leads to a potential underestimation of future EOL wood flows.

<heading level 3>Substance flows

Leaching approach:

For lead flows, the approach results in drastically higher estimates than the cross-checking values. The range of the result for chlorine is within the range of the standard deviation, but only because of the large uncertainty of the cross-checking value. Only for PAH flows does the mean value of the results lie close to the mean of the cross-checking value.. The problem from the goods level (through taking a leaching share of the aggregated stock as an output) is propagated. From a future perspective, even more inconsistencies arise at the substance level. As PAH, lead and chlorine were forbidden in 1996, buildings from earlier periods will also be free of contaminants after renovations. This is ignored by the leaching approach, leading to overestimated amounts of contaminants until the end of the modeling period.

Delay approach:

The substance flows may be slightly underestimated by the delay approach as the wood containing the substances often resides longer in stock than the technical lifetimes (cf. initial lifetimes of EOL wood flows). However, the cross-checking with data on substance flows in waste wood shows that (at present) the estimated amounts of substances lie within plausible ranges. From a future perspective, this approach is reasonable as all amounts of contaminants appearing after 1996 are only delayed outputs from previous periods. After renovations, where all wood constructions have been replaced, even old buildings will be free of these contaminants.

<heading level 1> Conclusions

For historical observations of EOL wood and its influence on current periods, the delay approach is a better choice than the leaching approach. Furthermore, the delay approach is also more representative at the substance level. For future predictions at the goods level, the delay approach should be adapted to consider the persistent share of historical buildings in the stock. These recommendations can be transferred to other dynamic analyses of building waste flows at a goods and a substance level under similar assumptions, particularly if forbidden contaminants are traced back and their influence on future periods is of interest.

Although the lifetime-driven delay approach is based on a lot of assumptions and the input of buildings has to be derived from incomplete data based on building census and assumptions about the building stock categorization, the results are more reliable than those of the leaching approach. Despite the fact that the use of the available data (data on building stocks, construction and demolition rates) to define the input to the leaching approach requires fewer assumptions, this modeling approach neglects the importance of diversity of the building stock (cf. van der Voet et al. 2002). The leaching approach assumes that all buildings in stock have the same likelihood of being demolished or renovated since renovations and demolitions are always considered for the aggregated stock. However, buildings from 1946-1976 are more likely to be demolished or renovated than buildings from 1997 onwards, which contain half of the wood content.

Overall, the most critical parameters in both approaches are related to the wood contents in buildings, which may differ extremely from one period to another. In order to get more realistic results using the leaching approach, the model would need to be extended so that the leaching part is not taken from the aggregated stock but is instead time-dependent, making such a study very resource and data intensive. However, this would be irrelevant in cases of a highly homogenous building stock. For studies which analyze EOL flows associated with buildings of very similar material intensity, the leaching approach is an adequate and easily applicable method, provided that reliable data on renovation and demolition activities (over time) are available.

The effect of the choice of lifetimes in the delay approach (such as the lifetimes of the historic stock in this case study) can also be adapted by modification of external parameters which extend the duration in stock by leaving the buildings in a depleted pool. For this case study, an extension parameter was introduced to consider the effect of the business cycle on building demolition and renovation. However, the consideration was purely didactic owing to a lack of data to derive meaningful parameter value estimates for the share which depends on this parameter in the delay approach. Therefore, future studies should consider such effects based on historic data and economic models.

<heading level 1> Acknowledgments

This research was carried out within the program “Innovative Projekte” of the TU Wien and the Christian Doppler Laboratory on Anthropogenic Resources, funded by the Austrian Federal Ministry of Science, Research and Economy and the National Foundation for Research, Technology and Development.

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Supporting Information

related to

Evaluation of modeling approaches to determine end-of-life flows associated with buildings: a Viennese show case on wood and contaminants

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This supporting information contains the formulas for the modelling approaches and assumptions which are made in the calculations. Furthermore, it contains detailed information and graphical interpretations of the sensitivity analysis results of the global and local sensitivity analysis used in the manuscript.

Contents

SI-1: Formulas for Modelling Approaches and Assumptions

The following section contains calculation steps which are done in the modelling approaches in a formalized way. While section a) and b) contain only the assumptions made in the respective approach, c) contains the assumptions which are valid for both approaches.

a) Leaching stock approach:

$O(t) = f(t, c + r)S(t)$……Total EOL wood flow output per year t (1)

$O_{sub}(t) = f(t, c + r)S_{sub}(t)$……Total Substance flow output per year t (2)

$S(t) = bs(t) \sum_{j=1}^{5} \sum_{i=1}^{6} a(t, j)cont(j)cat(j, i)$……EOL wood stock per year t (3)

$S_{sub}(t) = bs(t) \sum_{j=1}^{5} \sum_{i=1}^{6} a(t, j)cont(j)cat(j, i)\, sub(i, t)$……Substance stock per year t (4)

$c, r \in [0,1]$……demolition rate, renovation rate (5)

b) Delayed input approach:

$O(t) = \sum_{i=1}^{6} O_i(t)$……Total EOL wood flow output per year t (6)

$O_{sub}(t) = \sum_{i=1}^{6} O_{i_{sub}}(t)$……Total Substance flow output per year t (7)

$O_i(t) = pI_i(t - L_i) + f(t, 1 - p)I_i(t - L_i)$……Output flow of each product category i=1,.,6 (8)

$O_{i_{sub}}(t) = pI_{i_{sub}}(t - L_i) + f(t, 1 - p)I_{i_{sub}}(t - L_i)$……Substance flow output of each product (9)

$I_i(t) = bi(t) \sum_{j=1}^{6} \chi_{Mj}(t)cont(j)cat(j, i)$……Input flow of each product category (10)

$I_{i_{sub}}(t) = bi(t) \sum_{j=1}^{6} \chi_{Mj}(t)cont(j)cat(j, i)sub(i, t)$……Substance input flow of each product (11)

$bi(t) = \delta S(t) + bo(t)$……Input of buildings in stock per year t (12)

$\delta S(t) = S(t - 1) - S(t)$……Change in building stock per year (13)

$bo(t) = \sum_{j|t \notin M_j} [a(t, j)bs(t) - a(t + 1, j)bs(t + 1)]$……Output of building stock per year (14)

$\chi_{M_j}(t) = \begin{cases} 1, & t \in M_j \\ 0, & t \notin M_j \end{cases}$..Characteristic function of the set M_j identifying the building period of t (15)

$M_j = \{t \mid t \text{ is in the time period } j\}$……Set of years t which belong to time period j, j=1..,5 (16)

$L_i \in N$…… ……Lifetimes of product categories i, i=1,..,6 (17)

$p \in [0,1]$……share of buildings which do not depend on the business cycle (18)

c) Assumptions made in both approaches:

$f(t, d) = 0.0005\sin(\frac{\pi}{10}t) + d, f: N \times R \to R$……Business cycle function per affected share d (19)

$bs: N \to R$…… …… Building stock per year t (20)

$a: N \times N \to [0,1]$…… …Categorization of age classes j of building stock per year t (21)

$cont: N \to R$…… ….Wood contents for age classes per building j, j=1,..,5 (22)

$cat: N \times N \to [0,1]$…… ..Shares of wood products i in buildings of different time periods j (23)

$sub: N \times N \to R$……substance value per product category i per year t, i=1,..,6 (23)

SI-2: Local sensitivity analysis of EOL wood and substance flows

The sensitivity of the model outputs is tested by changing specific parameters one-at-a-time. The models were tested for the critical parameters renovation and demolition rate in the leaching approach and lifetimes in the delay approach. The results are given in 2.1. Furthermore, the EOL wood flows were tested for the crititcal categorization of wood stock parameters and the substance flows for the age of buildings which influence the output flows in current periods. The results are given in 2.2. and 2.3.

SI-2.1: Testing of renovation & demolition rate /lifetimes on EOL wood flows

Both, lifetimes and renovation plus demolition rate, show a linear behaviour with regard to the EOL wood output flows. Thus, changing the parameters changes the output flows in a linear way. Outputs from the leaching approach change directly proportional to changes in demolition and renovation rates, while outputs in the delay approach change indirectly proportional. An increase in lifetimes increases the material stock and decreases the output flows. The results of doubling the renovation and demolition rate and doubling the lifetimes are given in Figure SI-2.1.As it can be seen, doubling the renovation and demolition rate doubles the amount of output, while doubling the lifetimes halves the amount of output.

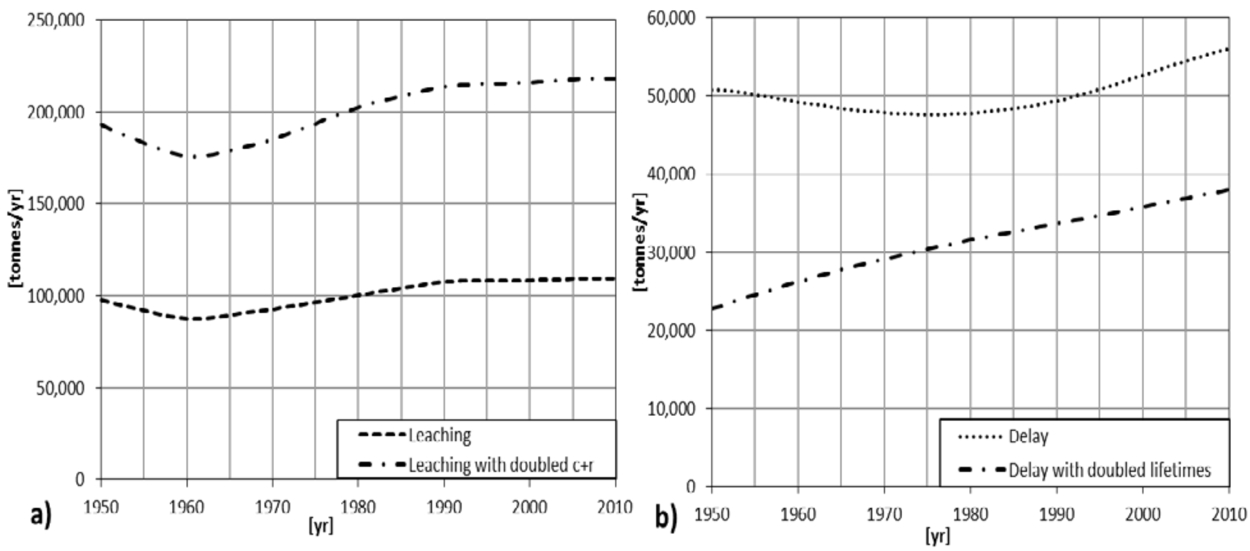

Figure SI-2.1: EOL wood flows for doubled renovation and demolition rate for the leaching approach (a), and doubled lifetimes for the delay approach (b).

SI-2.2: Testing of reallocation of wood stock on EOL wood flows

As the share of buildings –1918 is the highest in the Viennese building stock in for each period and as the wood amount per building is far higher than for each other period (see data in the manuscript), it is tested for sensitivity for the historical output until 2010. For the leaching approach, the share of stock of –1918 is decreased for 20% and this 20% are reallocated equally to all other periods in stock. For the delay approach, the initial share of 70 000 buildings containing 83% of buildings –1918 and 17% of 1919-1946, is redistributed to 50% each. The results are given in Figure SI-2.2. As it can be seen, this causes significant differences for both approaches.

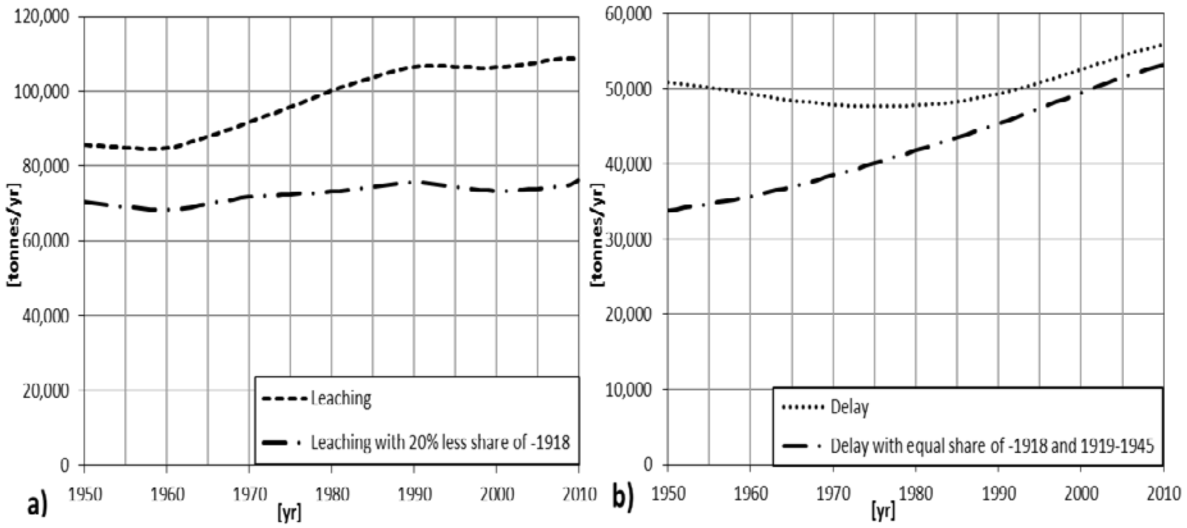

Figure SI-2.2: EOL wood flows for reallocated amounts of building stock for the leaching approach (a) and the delay approach (b).

SI-2.3: Testing of sensitivity of age of buildings on PAH flows

Here, the PAH output flows are tested for sensitivity with regard to input shares of the age periods (initial stock of -1918 and 1919-1945,1946-1976 and 1977-97) of the building stock. Each scenario leaves out one of the input shares. The results are given in Figure SI-2.3. It can be seen that in 2010, the most important contribution to the PAH output flows is given by the initial share of stock in the leaching approach and by the 1977-97 stock in the delay approach.

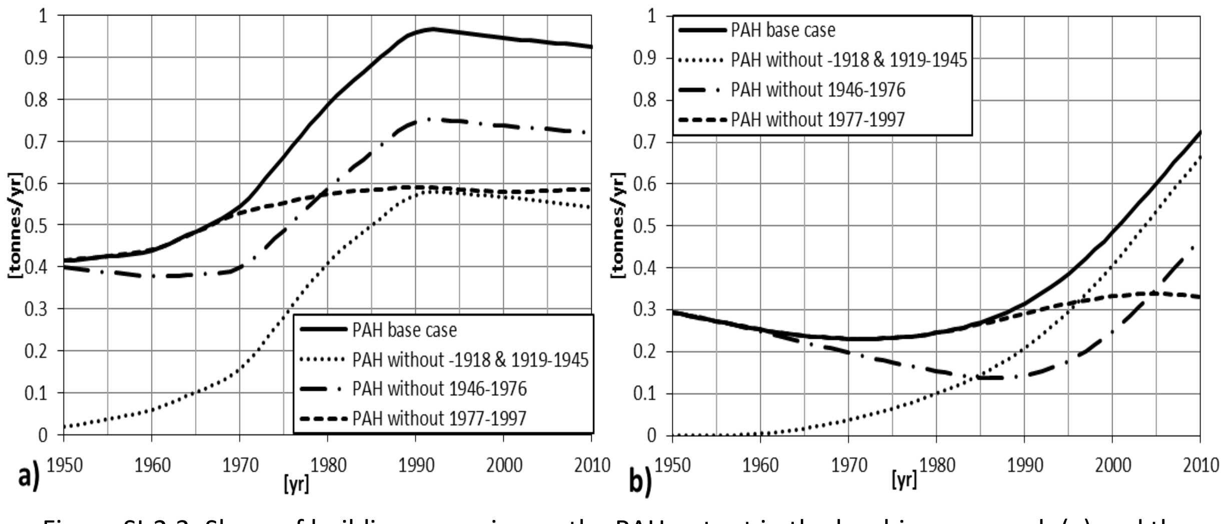

Figure SI-2.3: Share of building scenarios on the PAH output in the leaching approach (a) and the delay approach (b).

SI-3: Global sensitivity analysis of EOL wood and substance flows

The uncertainty of the model output is tested for its proportions of uncertain inputs. The analysis is done by using the EASI algorithm to find the sensitivity indices of first order (=without interactions with other parameters).

SI-3.1: Testing shares of wood inputs per building period on EOL wood flows

The sum of first order indices for the EOL wood output flow is less than 10% in both approaches, meaning that both models depend only on correlation effects of the parameters. Therefore, parameters were bundled to independent shares of input for each decade and the shares were tested for their first order indices.

In the leaching approach (see Table SI-3.1 a), the category of roofs has the main impact with in each year (slightly shrinking from almost 1960 on).The impact of ceilings varies around 20%. From the year 1990 on, the effect of floors is rising because the wood content of modern buildings is mainly given through floors. Some analogies can be observed for the observation of shares in the delay approach (see Table SI-3.1 b). Ceilings from -1918 (with technical lifetimes of 60 years) have the highest effect until 1990. From 1990 on, roofs -1918 (with technical lifetimes of 120 years) are dominant. Floors have an rising effect from 1980 on and they share is dominant in 2020.

a) Leaching	1950	1960	1970	1980	1990	2000	2010	2020
Windows	0.02	0.02	0.02	0.02	0.02	0.02	0.03	0.03
Roofs	0.73	0.78	0.73	0.67	0.62	0.61	0.60	0.60
Doors	0.01	0.01	0.02	0.02	0.02	0.02	0.02	0.02
Floors	0.01	0.01	0.01	0.08	0.14	0.17	0.18	0.18
Other wood products	0.01	0.01	0.02	0.03	0.03	0.03	0.03	0.03
Ceilings	0.23	0.20	0.22	0.20	0.19	0.18	0.19	0.19

b) Delay	1950	1960	1970	1980	1990	2000	2010	2020
Windows	0.10	0.08	0.07	0.05	0.05	0.05	0.07	0.09
Roofs	0.10	0.11	0.18	0.27	0.36	0.39	0.38	0.33
Doors	0.08	0.06	0.06	0.05	0.05	0.05	0.06	0.07
Floors	0.11	0.12	0.18	0.23	0.32	0.33	0.35	0.37
Other wood products	0.09	0.06	0.06	0.05	0.05	0.05	0.06	0.07
Ceilings	0.50	0.58	0.63	0.48	0.25	0.10	0.08	0.09

Table SI-3.1: Shares of first order indices for each decade for the leaching (a) and delay approach (b).

SI-3.2: Testing the input parameters on PAH, chlorine and lead flows

In a next step, parameters were tested for their first order indices of the output flows on a substance level. In these cases, there are high first order effects of the substance parameters. As the amounts of contaminants per product category are the only parameters with first order effects, all other parameters are ignored in the Figures in SI-3.2. It can be seen that for PAH flows, windows dominate the leaching approach until 1980, after that, floors have the highest first order indices. For the delay approach, we see that PAH amounts in floors have always the highest first order indices while the others are negligible. For the chlorine flows, chlorine amounts in ceilings have the only first order effects in the leaching approach, while in the delay approach, the amounts in ceilings are rather minor but the only effects of relevance until 2000. After 2000, chlorine in floors has the highest first order indices in the delay approach. Considering the lead amounts, we see that the only first order effects are given by floors in both approaches.

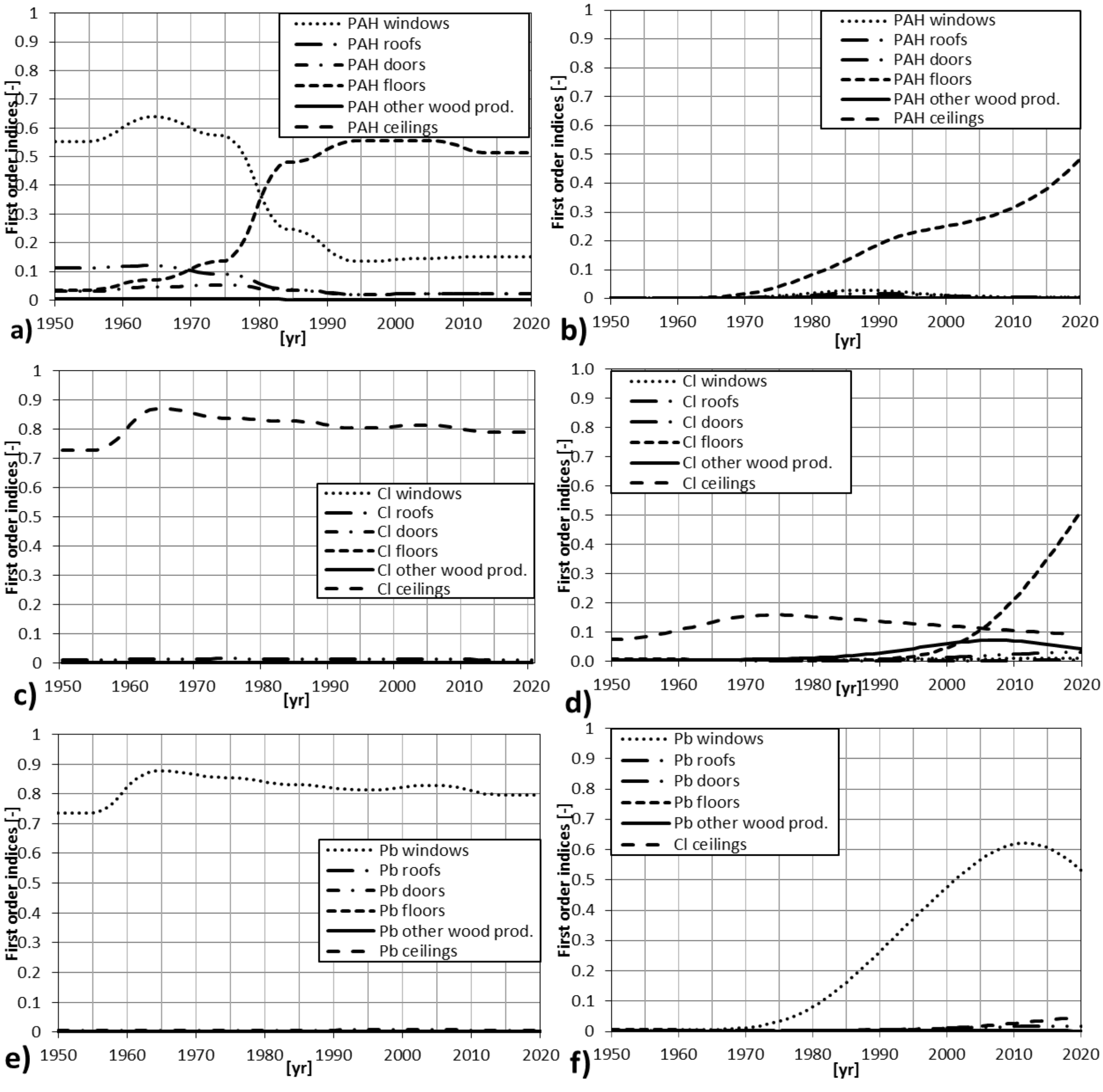

Figure SI 3.2. First order indices for PAH output flows in the leaching (a) and delay (b) approach, for chlorine flows (leaching (c) and delay (d)), and for lead flows (leaching (e) and delay (f)).