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Energy, Sustainability and Society

REVIEW

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Combining the worlds of energy systems and material flow analysis: a review

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Abstract

Recent studies focusing on greenhouse gas emission reduction strategies indicate that material recycling has a significant impact on energy consumption and greenhouse gas emissions. The question arises how these effects can be quantified. Material recycling is not at all or insufficiently considered in energy system models, which are used today to derive climate gas mitigation strategies. To better assess and quantify the effects one option would be to couple energy system models and material flow models. The barriers and challenges of a successful coupling are addressed in this article. The greatest obstacles are diverging temporal horizons, the mismatching of system boundaries, data quality and availability, and the underrepresentation of industrial processes. A coupled model would enable access to more robust and significant results, a response to a greater variety of research questions and useful analyses. Further to this, collaborative models developed jointly by the energy system and material analysis communities are required for more cohesive and interdisciplinary assessments.

Keywords: Energy system modeling, Material flow analysis, Recycling, Model coupling

Introduction

National energy systems must change drastically in order to be able to supply low-carbon or zero-emission energy in the future [1]. This change includes the advancement of renewable energy sources and their optimal integration into energy systems. Additionally, all end use sectors must achieve more sustainable development. In order to analyze the residential, industrial, transport, trade and commerce and power sectors, and to evaluate their influence on energy use and CO_2 emissions, energy system models must include these domains in their assessments [2]. Analyzing energy system models will help illuminate future energy supply and demand structures and enable assessment of the impacts of policy measures, e.g., CO_2 emission reduction targets, on different sectors [3]. The industrial sector is an especially important end use sector due to its energy intensity and high CO_2 emissions.

The study, 'The Circular Economy—A Powerful Force for Climate Mitigation' [4] comes to the conclusion that demand side measures can cut CO_2 emissions from the European industrial sector by almost 300 million tons per year by 2050. Materials recirculation opportunities alone contribute with ~60% to those savings (Fig. 1). To assess this energy saving and CO_2 mitigation potential the study used exogenously predefined recycling quotes, rather than making the recycling process part of the simulation or optimization used for the study. This practice gives little information on whether recycling is the right choice as a CO_2-reduction strategy. However, the effect of recycling on energy use and CO_2 emissions appear to be significant and deserve to be further holistically analyzed.

Recent publications suggest that the transition of the energy system goes hand in hand with a change in material flows and stocks. Grandell et al. analyze how clean energy technologies influence the market of critical resources in the future [5]. Rare earth elements, the embodiment of critical resources, refer to 17 elements

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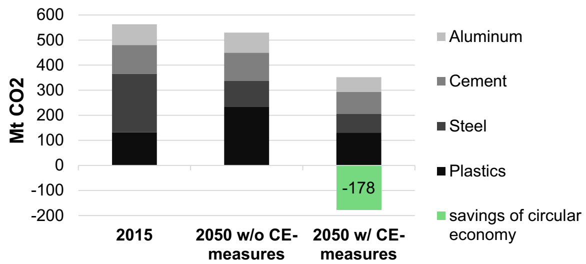

Fig. 1 Impact of circular economy (CE) measures on CO_2 emissions of industrial production within the EU. Illustration based on Material Economics, 2019 [4]

which are important for innovative digital and many low-carbon technologies [6]. Henckens et al. estimate market price trends of resources and future resource scarcity due to a trend towards innovative technology [7]. Kavlak et al. analyze the future metal demand in light of increasing photovoltaic expansion [8]. Lacal-Arántegui makes a similar estimation in regard to electricity generation by wind turbines [9]. Moss et al. analyze risks of potential metal supply bottlenecks for several energy technologies required for strategic future energy system designs [10]. On a national level, Viebahn et al. estimate the need for critical resources for the German energy transition [11]. Månberger and Stenqvist [12] link the energy system transition to an inevitable change in the entire resource and material supply chains. Consequently, they highlight the importance of recycling, not in relation to possible energy consumption but in light of resource availability. Tokimatsu et al. [13] conclude that modelers and policymakers should include material availability and varying production rates into their planning and modeling of future sustainable energy systems. Therefore, a more detailed look into recycling technologies and infrastructures is necessary to holistically evaluate the transformation of energy systems. Comprehensively modeling industrial processes in energy system models is one part of a systematic approach to representing energy use related to material flows and stock changes. Integrating material flows into energy system models could lead to a more consistent assessment, and thus to more salutary policy outcomes.

Material flow analysis (MFA) is a widely used assessment tool to evaluate policies and their impact on anthropogenic material cycles. Brunner and Rechberger [14] describe MFA as the systematic accounting of the flows and stocks of materials within a given system. This methodical approach is based on the law of conservation of matter and calculates a material balance for specific points in time within a given space [14]. There are static and dynamic MFAs for the assessment of anthropogenic material flows. A static MFA analyzes material flows and stocks at a time scale of one specific point and provides information in the form of a snapshot. Dynamic MFA, however, makes estimations of past and future flows and stocks as well [15]. Therefore, a dynamic approach can, for example, be used as an investment decision tool for future waste management infrastructures, or it can indicate whether future resource demands can be met [16].

Utilizing natural resources and transforming nature has feedback on society [17]. As a result, researchers such as Krausmann et al. [18] assess the development of global material use, gross domestic product and population in order to analyze resource use intensities. Pearce and Turner [19] were one of the first to directly connect natural resources and the economy, and eventually initiated the concept of the circular economy (CE). This notion has attracted great interest lately and is anchored in several European (e.g., an EU action plan for the circular economy [20], a European Strategy for plastics in a circular economy [21]) and national [22] policies, which influence the industrial sector. Geissdoerfer et al. [23] describe the core concept of a circular economy as a 'regenerative system' that focuses on minimizing resource and energy use, as well as the generation of waste and emissions. Closing material and energy loops via suitable end-of-life treatments of products is the main aim while switching from a linear 'take, make and dispose' model to a circular economy [24]. Suitable end-of-life strategies include reusing, repairing, remanufacturing and recycling products at the end of their lifetimes. In the literature, these strategies are called the '3Rs' principle, comprising *reduction*, *reuse* and *recycling* [25]. Several recent studies address the circular economy principle, specifically in relation to recycling and material efficiency.

The International Energy Agency (IEA) includes material efficiency and recycling strategies in its future scenarios that result in reductions of CO_2 emissions and energy use [26]. Institutes of the Renewable Energy Research Association state that recycling processes and the economical use of materials are prerequisites for realizing a low-carbon energy system in Germany [27]. Gerbert et al. [28] conclude that higher recycling rates of non-ferrous metals could lead to savings of up to 2 Mt CO_2-equivalent in Germany per year. Another study [29] calculates GHG emission savings of scrap-based, non-ferrous metal production to be 7 million tons, with higher potential through 2050. These studies suggest that circular economy measures and, specifically, material recycling seem to have a significant impact on energy use. These measures, however, are not equally advantageous for all materials. Ghisellini et al. [30] state that recycling is not beneficial per se and could become environmentally and economically unviable at a certain point.

Several studies have extended material flow models by the addition of economic parameters, enabling them to evaluate material strategies on a multi-criteria level [31] or to integrate economic decision-making into material strategy assessment [32]. Elshkaki et al. for example, analyze both environmental and economic effects of lead stocks in the Netherlands [33]. Dellink and Kandelaars estimate how fiscal policies for dematerialization influence material flows [34]. The consideration of additional flow parameters, however, also carries data-related challenges. Hawkins et al. [35] found that a more detailed estimation of material flows, a benefit of coupling economic flows with a material input output model, comes at a cost of greater data uncertainty. Furthermore, Streicher-Porte et al. [36] address the problem of data availability and quality when combining material and economic flows. Recent studies in the energy system modeling community analyze the effects of combining energy system models and lifecycle analysis to widen the system boundaries and include further sustainability goals [37]. In this regard, Pehl et al. used the integrated assessment model REMIND and found that the additional consideration of emissions embodied in energy technologies has only minor effects on future global energy scenarios [38]. Rauner and Budzinski develop a framework to feed an energy system model with input data of the ecoinvent database to optimize future energy system designs based on multiple objectives [39].

With the help of existing material flows and stocks, an energy system model, specifically of the industrial sector, could illustrate additional effects and provide more detailed insights. This paper analyzes existing material flow and energy system models. The focus is on how and to what extent these models incorporate circular economy principles. Further objectives of this paper are to demonstrate the benefits, threats and opportunities of combining material flow analysis and energy system models. The following question is addressed: Which challenges complicate a successful integration of material flow analysis and energy system models?

Some studies make statements or predictions about future energy demand or emissions related to recycling measures. Tokimatsu et al. for instance, use a bottom-up energy model to analyze metal intensities of three cost-optimal scenarios, which all satisfy the well-below 2 °C climate policy target [40]. However, these studies which assess the linkage between the energy transition and material flows, primarily focus on critical material demand and supply for future low-carbon energy systems and identify potential future bottlenecks in critical material supply. Although an assessment of varying recycling rates on security of supply of rare metals to achieve wind turbine or photovoltaic expansion is usually done, but the effects of recycling on the energy system design itself is lacking. There has been no systematic evaluation of the effects of recycling on future energy system designs, by means of cost-efficiency or effectiveness to reach climate goals, in competition with other climate gas reduction strategies. Consequently, there is no existing energy system model that can comprehensively evaluate the impacts of recycling. The theory of circular economy includes several more concepts besides recycling. Intensity of use, product and material lifetime, re-use, re-manufacturing, or for example material substitution are all ideas to either actively turn a linear into a circular economy or to measure the present circularity of an economy [23]. Since recycling is already a widely used practice, efficiencies, energy demand or costs of recycling processes can be quantified based on real-life data, and thus easier implemented in energy system models. Furthermore, as mentioned before, the effect of recycling on energy use and CO_2 emissions appear to be significant, and thus interesting to the energy system model community. Therefore, this review focuses on the recycling concept only. This paper offers insight into both material flow and energy system modeling and, for the first time, initiates conceptual dialogue between the two perspectives. In order to answer the above-mentioned questions, the following chapter explains how previous literature reviews have independently classified and analyzed material flow and energy system models. The methodology chapter also explains how the investigated models were chosen and which criteria for classifying and reviewing them were used. The classification of MFA and ESM, as well as the challenges of combining them, is given in the results chapter. A discussion of these results and conclusions follows this.

Literature review and model selection

Previous literature reviews on material flow analysis models have focused on the geographical coverage of MFA models [41], the link between MFA models and sustainable development [42], as well as the methods used in dynamic material flow analysis [15] (see Table 1). According to Huang et al. [42], the integration of material flow and lifecycle assessment, as well as the use of material flow analysis, together with risk assessment are interesting potential future research

Table 1 Recent reviews of material flow and energy system models

	Author	Investigated models	Focus
Material flow models	Müller et al. [15]	60	Material dissipation, spatial dimension, data uncertainty
	Huang et al. [42]	150	Relationship between material flow analysis and sustainable development
	Bao et al. [41]	129	Spatial horizon and methodology
Energy system models	Ringkjob et al. [47]	75	Model capabilities and future challenges
	Lopion et al. [48]	24	Methodology, time/space resolution, modeling language, time horizon
	Pfenninger et al. [2]	100	Time/space resolution, uncertainty, complexity, human behavior
	Pauliuk et al. [45]	32	Integration of industrial ecology measures in integrated assessment models

topics. However, the authors also state that the coupling of material flow analysis with other sustainable development tools is threatened by data availability and uncertainty [43]. Pesonen [44] investigated the combination of material flow models with economic decision-making concepts. Meanwhile, Pauliuk et al. [45] investigated how industrial ecology measures can be incorporated by integrated assessment models. They reviewed five integrated assessment models (IAM), of which only one (IMAGE 3.0) had partly implemented material cycles. Pauliuk et al. concluded that the integrated assessment modeling community must better document its models, especially the interfaces, and extend their oft-isolated toolboxes so as to achieve a successful combination of industrial ecology and integrated assessment models. The pathway towards Open-X modeling can be one solution to overcoming this challenge [46].

The coupling of models can be undertaken in two distinct ways, with either the 'soft' or 'hard' coupling of two or more models. Soft coupling is defined in this paper as the process of running both models separately and using the output from one as the input for the other. This can be performed either once or through the iteration of multiple periods. Hard coupling, on the other hand, is understood as the simultaneous running of multiple interlinked models, with variables of the different models used in a closed modeling system. Beaussier et al. [49] state that usually, the more complex and advanced model spans the spatial extent and time frame, as well as the technical aggregation level of the coupled system.

The interconnection of material use and energy system design is, for instance, discussed in Månberger and Stenqvist [12]. They explicitly analyzed the demand for 12 metals and how this is affected by the energy conversion technology mix, as well as different energy scenarios. They showed that the choice of energy conversion technology (e.g., photovoltaic) has a major impact on the demand for specific metals. Lang et al. [50] coupled material and money flows to more comprehensively assess the recycling industry; an approach that enabled questions regarding the feasibility of recycling processes to be answered. They found that integrating economic data into material flow analysis leads to more robust results and improvement strategies. Boubault et al. use the TIMES integrated assessment model and estimate future material demands necessary for the expansion of energy technologies to reach the well-below 2 °C target [51]. Solé et al. introduce a new open-source energy system model and include constraints for raw materials needed for the renewable energy transition in order to consider material scarcity effects [52]. Another study that estimates material and energy investments in technologies of renewable energy transition scenarios is conducted by Capellán-Pérez et al. [53]. Allwood et al. state that recycling is an effective measure to decrease energy demand and thus CO_2 emissions for the global production of steel, cement, plastics, paper and aluminum [54] Milford et al. focus on the steel industry and state that emission targets can only be reached by a combination of energy and material efficiency measures [55]. Van der Voet et al. summarize the linkages between materials and energy and the importance of paying more attention on feedback loops between the two research fields [56]. A further study by Kleijn et al. stresses the interconnection of materials and energy systems and found that a transition towards low-carbon power generation would require significant amounts of metals [57]. Watari et al. analyze the scenarios of the international energy agency and state that recycling of critical metals is necessary to achieve the proposed expansion of renewable energy technologies [58]. In other studies, Watari et al. estimate material requirements for the global transport and electricity sector until 2050 [59] and specifically analyze how circular economy measures support security of supply of lithium for applications in electric vehicles [60]. Giurco et al. reinforce the previous findings and state that increased recycling rates can support the transition presented in 100% renewable scenarios [61]. Rauner and Budzinski [39] proposed broadening the currently implemented understanding of sustainability in energy system models by conducting a lifecycle assessment. With this approach, they also call for a joint collaboration of energy system modelers and the industrial ecology community. Such a model coupling avoids shifting of the problem and accounts for otherwise neglected trade-offs. Coupling energy system and material flow models can help in assessing how circular economy measures (e.g., recycling quotes) influence material availability and the energy system's design. Research questions arising include how the availability and quality of material flows and stocks influence the energy system design, and vice versa. A coupled energy system and material flow model can answer these and assess related material and energy policies.

Criteria for model selection

The review articles cited in Table 1 stay in the realms of their field (materials or energy) and do not consider the criteria of the contrasting research area for analyzing their models. This paper combines a review of the models of both research fields for the first time. For the selection of appropriate models, the following eligibility criteria were applied.

Eligible material flow models must have at least a regional perspective on their investigated material. Assessments of single industrial processes or product chains with no relation to a suitable spatial system boundary are not considered. Only prospective material flow models are considered and retrospective discarded. Due to their nature of merely accounting for historic material flows and stocks these retrospective approaches will not be reviewed in detail. Their lack of estimation for future developments makes them impractical for analyzing effects of recycling on future energy system designs. With prospective material flow analyses and suitable exogenous assumptions on future material demand and supply, estimations about future scrap availability can be made [62], which is necessary to analyze the development of recycling in the context of an energy system. In addition to structural prerequisites, certain requirements concerning the transparency of their documentation are set up. The use of the model and the related input data have to be documented in such a way that it is possible to compare the data of the different models to each other. Furthermore, the study has to explain in detail which domains are included in the model scope, so that a comparison of whether energy flows are part of the material flow analysis is possible. This paper reviews 52 material flow models.

Based on recent energy model reviews by Ringkjob et al. [47] and Lopion et al. [48] the following criteria were applied to find suitable energy models. Eligible energy system models must cover all energy demand sectors (electricity, heat, transport, industry goods) and provide sufficient documentation of their methodological approach. In order to have a representative methodological analysis, simulating as well as optimizing energy system models are chosen. At least one model each that covers national, sectoral and global energy systems is selected to be able to compare them with the respective material flow models. Each model must have a detailed implementation of the industry sector, which provides the interface between the material and energy domains. For both material flow and energy system models applies that they must be able to support governments in decision-making related to resource use or energy system design, respectively. The type of assistance or governmental decision-making can vary, depending on the research question, from analysis of policies of mandatory recycling quotas to climate gas mitigation strategies of a country. As an example, measures within the recently released 3rd version of the program for resource efficiency [63] by the federal government of Germany have no direct relation to energy use or CO_2 mitigation strategies. However, an integrated consideration of both resources and energy could provide important insight for decision-makers. As a consequence, for the purpose of better understanding the environment needed for integrating recycling into energy system models as one part of the industrial ecology thinking [64], these five energy system models are selected; FORECAST, CIMS, NEMS, ESME and TIMES-TIAM. The authors intentionally do not consider integrated assessment models (IAMs), since a significant amount of research on the topic of combining IAMs and circular economy measures has already been done. Pauliuk et al. analyze prospective models and state how IAMs can benefit from industrial ecology measures [62]. In a more recent work, Pauliuk et al. review IAMs and assess how industrial ecology can be integrated [45]. Boubault et al. use the TIMES IAM and integrate life cycle inventories [65]. Capellan-Perez introduce the MEDEAS integrated assessment modeling framework and the connection of materials and energy within the model family [66]. Nevertheless, since integrated assessment models have energy system models at their core, recommendations made in this article related to progressions of ESMs apply equally to IAMs.

Classification and evaluation of material flow and energy system models

To assess the prerequisites for the successful combination of material flow and energy system models, the models are classified regarding their system boundaries, methodology, spatial and temporal extent, as well as scope. Subsequently, the classified models are compared to evaluate coupling possibilities and constraints.

Material flow models

Material flow models describe how materials are drawn from nature into the anthroposphere as inputs, how they are manufactured into products and byproducts, and how waste and emissions flow back to nature [67]. A typical goal of MFAs is how certain material flows affect waste streams or how, in dynamics MFAs, consumption behavior affects resource stocks over time. MFAs are modeled for small regions [68], on a national scale [69] and at the global level [70], but foremost for a single specific material or product group only [71]. Depending on the scope of the study, MFAs are used for industrial process assessment, policy evaluation or large-scale environmental assessment.

Underlying methodology

Every material flow model is based on the systems approach and the principle of conservation of mass. Ayres and Kneese [72] were the first to establish a nation-wide material flow accounting for the USA. Their primary reason for developing such a systematic accounting approach for material flows was purely economic. The fact that society can consume environmental goods, like water and air, for free, consequently making them scarcer, disturbs the pareto-optimal allocation of these and other goods on the market. This systems approach is also described by Fischer-Kowalski [73] as "society's metabolism." Accompanying the systems perspective, each MFA is bound to conservation of mass [74]:

$$\textit{Material Input Into The System} = \textit{Material Output} + \textit{Changes In Material Stocks}. \tag{1}$$

As a quantitative process for calculating material flow and stock dependencies [75], the basic underlying methodology of an MFA is a matrix with in- and output flows, as well as with accumulating or shrinking stocks. This makes the base structure of any MFA a simple case of accounting of the material and goods within a system [76]. Müller et al. [15] describe retrospective and prospective top-down and bottom-up approaches to employ this accounting method. Retrospective and dynamic approaches are past-oriented flow analyses of several years. Du et al. for instance calculate global stocks of rare earth elements with past flow data [77], and Bonnin et al. analyze past copper flows and stock accumulation in France [78]. Prospective approaches, on the other hand, use flow data to predict future material flow relations and stock accumulation. Koning et al. for example try to estimate whether future low-carbon economies are limited by metal supply constraints [79]. Schipper et al. try to assess the future global copper demand in 2100 [80]. Of all the reviewed MFAs, the most frequently used is a combination of both approaches, where past flow and stock data are used to determine possible future states. Parajuly et al. for example predict future flows and stocks of waste electrical and electronic equipment [81] Choi et al. assess the development of indium flows in relation to increasing expansion of innovative technologies [82]. Another distinction between MFAs is whether these models are static or dynamic. Static models analyze a present snapshot in time, and do not consider flows between different time steps (cf. [83]), but most reviewed models analyze flows of several years and the interdependencies between these.

Scope

Material flow models focus on either individual substances, materials, compound products, whole process chains, or combinations of these. The majority of material flow models analyze the changes of flows and stock accumulation of individual elements and materials over time to illustrate the basic material cycle and assess resource availability. Giljum et al. for instance, calculate the material footprint for several countries worldwide [84]. Whereas Khonpikul et al. analyze the whole supply chain for feed production on a national level in Thailand [85]. Some models analyze scrap generation and future scrap availability to determine possible recycling quotas and evaluate current recycling procedures. Buchner et al. analyze future supply and demand of copper scrap in Austria [86], and Wang et al. assess copper scrap flows in China [87]. Gauffin et al. study the steel flows in the United States and estimate circulation flows of steel scrap in certain industry sectors [88]. Daigo et al. focus on recycling processes for waste ceramics and glass and try to optimize efficiencies [89]. Wang et al. [90], for example, observe global steel flows and specifically analyze how manufacturing affects the circular economy in the steel-making process. Golev and Corder [91] assess metal flows in Australia and illustrate metal scrap generation, collection and recycling rates. Zhang et al. [92] analyze copper flows and stock changes in China, stressing the importance of scrap utilization in the future copper economy. Some models focus solely on the material itself and quantify the flow and stock accumulation to illustrate their changes in a given region over time. Issues of interest are for example flows of nano-titanium particles [93] or carbon nanotubes in Switzerland [94], phosphorous flows in Austria [95], neodymium magnets in Denmark [96] or recycling potentials of indium in Europe[97]. Wiedenhofer et al. [98], as well as Heeren and Hellweg [99], analyze future flows and stocks of construction material. Xue et al. [100], meanwhile, solely focus on refrigerants in the household air conditioner sector and describe the flows of these in Japan through 2050. Wang et al. [101], in turn, count iron and steel stocks in China and predict future iron and steel dynamics. Fishman et al. [102] analyzed socio-economic drivers and how these affect the dynamics of stock accumulation. Another major share of the reviewed models evaluates end-of-life treatments of selected elements or materials to evaluate state-of-the-art technologies and derive policy recommendations. Allesch and Brunner use material flow analysis to improve waste collection and treatment for selected goods and elements in Austria [103]. Tazi et al. analyze waste streams of obsolete French wind energy plants to derive end-of-life treatment strategies [104]. Van Ewijk et al. observe global pulp and paper flows and assess their recycling rates based on sustainability [105]. Pfaff et al. [106] analyze copper flows in Germany to assess material efficiency measures. Few models assess whole product chains rather than individual elements or materials and thus focus mainly on in-use flows and stock changes. Valero Navazo et al. calculate flows and stocks of material recovery processes for obsolete mobile phones [107]. Bobba et al. focus on reused batteries and how the accumulate in the European Union [108].

Although elements within the rare earth elements group (REE) are not per se related to emissions or energy use, they are of great relevance for future energy system design [109]. Therefore, material flow models that focus on these elements already have a connection to the energy system's design. Of all the analyzed material flow models, 15 focus on REEs (see Table 2). Fishman and Graedel [110] analyzed neodymium flows in the United States, with their dynamics relating to the construction of offshore wind power plants. Sun et al. [111] analyze the dynamics of lithium flows for the electrification of the transport sector and conclude that efforts towards more efficient recycling technologies must be undertaken to secure a sufficient lithium supply in the future. Another energy system-related problem is addressed by Glöser et al. [112]. They analyze the raw material criticality and dynamics of Japan and Germany as two import-dependent economies. Also, Thiébaud et al. [113] observe REE flows and their routes in relation to electronic equipment in Switzerland. More related to future energy system design is the study by Yokoi et al. [114], in which is analyzed the dynamics of mineral resources depending on primary resource use changes.

Spatial and temporal extent

The following section illustrates the spatial and temporal extent of all models and the assumptions they make concerning the future dynamics of material flow and stocks. Most of the models assess material flows at a national level (see Fig. 2) while only one of all the reviewed models quantifies the flows and stocks on a communal scale. Dzubur et al. [68] compare different modeling approaches to account for secondary raw material flows in the Viennese wood construction sector. They point out that varying the wood content in different construction periods increases data uncertainty and complicates

Table 2 Elements and materials covered in the 52 reviewed material flow models

Material/product	Considered in no. of models
Rare earth elements	15
Copper	10
Steel/iron	7
Cement	7
Aluminum	7
Phosphorus	2
Nano-particles	2
Wood	2
Various (paper, glass, refrigerants, plastics, batteries, etc.)	5

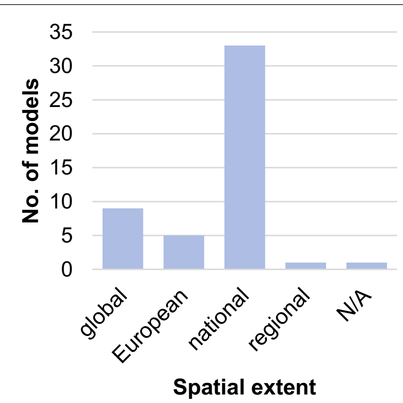

Fig. 2 Models by spatial extent

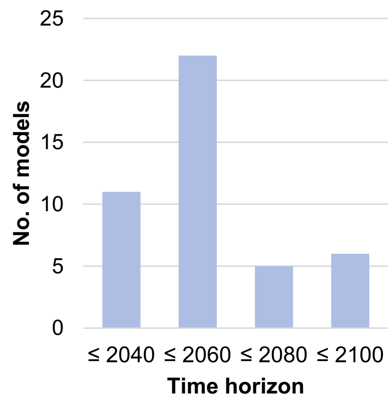

Fig. 3 Models by time horizon

predictions of future secondary wood flows. The models that analyze global material and element flows usually focus on the material itself and assess the change of resource availability and use over time [115]. Krausmann et al. [116] analyzed the global accumulation of material stocks from 1990 to 2010 and found that only 12% of inflows to these stocks, mainly infrastructure and buildings, derive from secondary material flows. Only five of the assessed models quantify flows at a European level.

Material flow models either assess past material flows and stocks (retrospective), make predictions of future flow and stock changes (prospective), or combine both approaches. As explained earlier this paper focuses on models that include prospective analyses only. Bader et al. [117] model both retrospective and prospective copper flows and stocks in Switzerland from 1850 to 2050, whereas Schipper et al. [80] estimate global copper flows until 2100. The majority of models, however, set their time horizon until 2060 (see Fig. 3). Crucial for predicting future material flows over long periods is the assumed lifetime distribution for materials and products residing in stocks. The majority of the analyzed models use a Weibull or normal distribution, which is in accordance with the findings by Müller et al. [15].

System boundary

Among all of the reviewed models, elements of the REE group, the bulk metals of copper, steel, aluminum and cement are the most frequently analyzed (see Table 2). The extraction and production of these metals are related to significant energy use and CO_2 emissions, thus highlighting their impact on energy system design. Metals make up more than 60% of all considered materials and only a few models investigate the flows and stocks of non-metals. Geyer et al. [118], for example, analyze global plastics flows and stocks, while Daigo et al. [89] evaluate the recycling strategies of glass in Japan. Van Ewijk et al. [105] assess the global end-of-life treatments of paper products, while Taulo and Sebitosi [119] evaluate tea production in Malawi. The models assess material flows in the product categories of general construction (e.g., construction sector in Japan [120] or housing in China [121]), infrastructure (e.g., cement for infrastructure in China [122]), transportation (e.g., aluminum use in future vehicles [123]), agriculture (e.g., phosphorous application in Denmark [124]), clothing (e.g., plastics in textiles [125]) and electronic equipment (e.g., end-of-life treatment of business devices [126]). In principle, all MFA models follow the generic systematic approach as seen in Fig. 4. Narrowing down the system boundary allows a focus on specific phases of the material cycle in more detail, whereas stretching the system boundary enables consideration

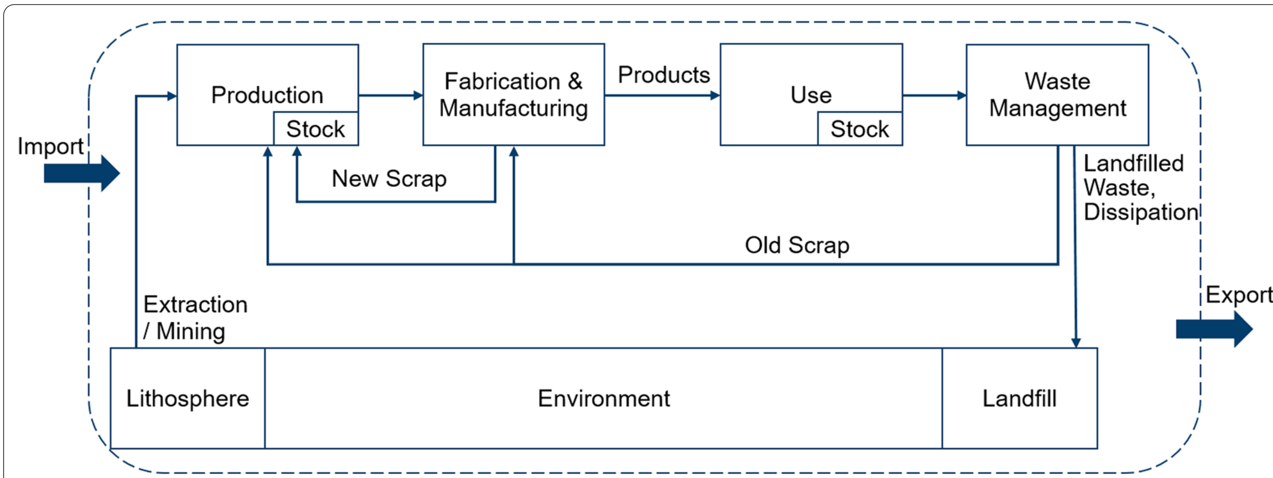

Fig. 4 Visualization of a generic MFA based on Laner and Rechberger [127]. The dashed line represents the system boundary

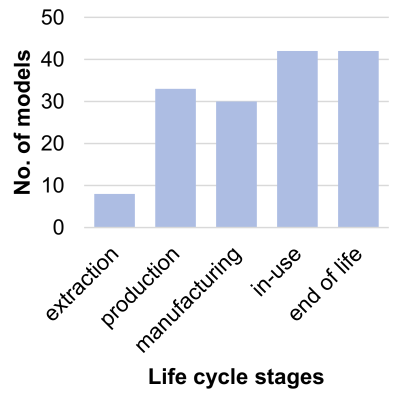

Fig. 5 Models by system boundary

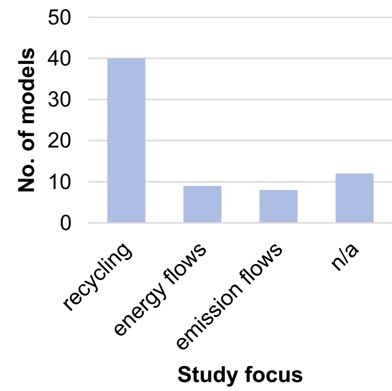

Fig. 6 Models by study focus

of adjacent systems as well. For example, focusing on the extraction of iron ore allows deeper analyses of processes in iron ore mines, related infrastructure and management of overburden material and waste water. Assessments of the production of steel or other related lifecycle phases require a broader system boundary and may lead to less detailed analysis of the extraction lifecycle phase due to increased complexity.

Almost all of the reviewed models applied this generic approach of balancing material flows from extraction over production, manufacturing, use-phase to waste management, and accounting for stocks in all phases. Most of them focus on the in-use and waste management phase (44 studies), with more than 30 models considering the production and manufacturing phases. The mining and extraction of raw materials is not regarded as important (see Fig. 5). The greatest share of models analyzed recycling processes, material waste flows and secondary raw material flows. However, only a minority accounted for energy or emission flows (see Fig. 6). Among these, two models partially analyzed energy flows in relation to energy system models. Morfeldt et al. [128] used a model to assess steel scrap availability and fed the results into the global energy system model, ETSAP-TIAM, to analyze the impacts of global climate targets on the choice of steel production technology. Van Ruijven et al. [129], meanwhile, integrated a cement and steel model into a long-term global integrated assessment model (IMAGE) to predict future CO_2 emissions and energy use in the steel and cement industries. They conclude that there is huge potential to reduce CO_2 emissions in the steel and cement industries with a carbon tax of 100 $/tCO_2$. Apart from those two models, no other reviewed model considers the interactions of material cycles and energy system models.

Energy system models with an implemented industry sector

Energy system models (ESM) are either be used to describe and evaluate the current state of an energy system or to create future scenarios of it [130]. The goal is to describe the system in its entirety, from energy carriers through energy transformation technologies, transmission and storage media, to the implementation of different energy-intensive sectors, such as transportation and heavy industry. The scope of energy system model analysis has changed over time, from risk assessment of national energy supply and environmental assessment of energy systems, to the evaluation of volatile renewable energy technologies [48]. ESMs are both programmed for the simulation of contemporary and future energy systems, as well as for the optimization of future energy systems and the transmission paths leading to that state. These models can be used for multi-regional as well as single-node calculations and can cover a wide spatial and temporal scope. Common goals are policy implications and the evaluation of the total system design. The following energy system models were chosen on the basis of the availability and accessibility of data, as well as sufficient documentation of modeling methodologies. Specifically, as the reviewed models are under continuous development, the presented results show the state of each model at which the model itself or an additional, related feature was published.

Model		FORECAST [131]	CIMS [132]	ESME [133]	NEMS [134]	ETSAP-TIAM [135]
General model parameters	Methodology	Simulation	Simulation	Optimization	Simulation	Optimization
	Spatial extent	1-node (Germany)	1-node/multi-regional	Multi-regional (UK)	Multi-regional (USA)	Multi-regional (global)
	Temporal resolution/time horizon	1 year/until 2050	5 years/2005–2030	2 seasons, 5 intraday times/2010–2050	9 segments/flexible, through 2050	Typical days, hours/flexible
	Considered sectors	Electricity, heat, transport, industry	Electricity, heat, transport, industry	Electricity, heat, transport, industry	Electricity, heat, transport, industry	Electricity, heat, transport, industry
	Considered industrial branches	Iron and steel, non-ferrous metals, paper and printing, non-metallic mineral products, chemical industry, food, drink and tobacco, engineering and other metal, refineries, other non-classified	Chemical products, industrial minerals, iron and steel, metal smelting, metals and mineral mining, other manufacturing, pulp and paper, petroleum refining	Iron, steel and non-ferrous metals, chemicals, metal products, food, drinks and tobacco, paper, other industry, agriculture, refined petroleum products	Detailed modeling of process flows for glass, cement and lime, aluminum, iron and steel, pulp and paper	Agriculture, food and tobacco, chemicals, metals, cement, bricks, glass, other commodity production, wholesale and retail trade, private service, construction, other utilities, motor vehicle purchases and repair
Circular economy parameters	Material flows	Not considered	Not considered	Not considered	Not considered	Not considered
	Recycling	Recycling quota for materials is based on exogenous assumptions	Not considered	Not considered	Recycling quota for materials is based on exogenous assumptions	Recycling quota for materials is based on exogenous assumptions
	Costs	No costs included for recycling technology and recycling infrastructure	No costs included for recycling technology and recycling infrastructure	No costs included for recycling technology and recycling infrastructure	No costs included for recycling technology and recycling infrastructure	No costs included for recycling technology and recycling infrastructure
	Waste/end-of-life treatment	No/extremely aggregated consideration of waste management	No/extremely aggregated consideration of waste management use of waste wood in industrial sector	No/extremely aggregated consideration of waste management	No/extremely aggregated consideration of waste management	No/extremely aggregated consideration of waste management
	Material substitution	Exogenous assumptions/aluminum or carbon fiber use in vehicle construction	Not considered	Not considered	Not considered	Not considered

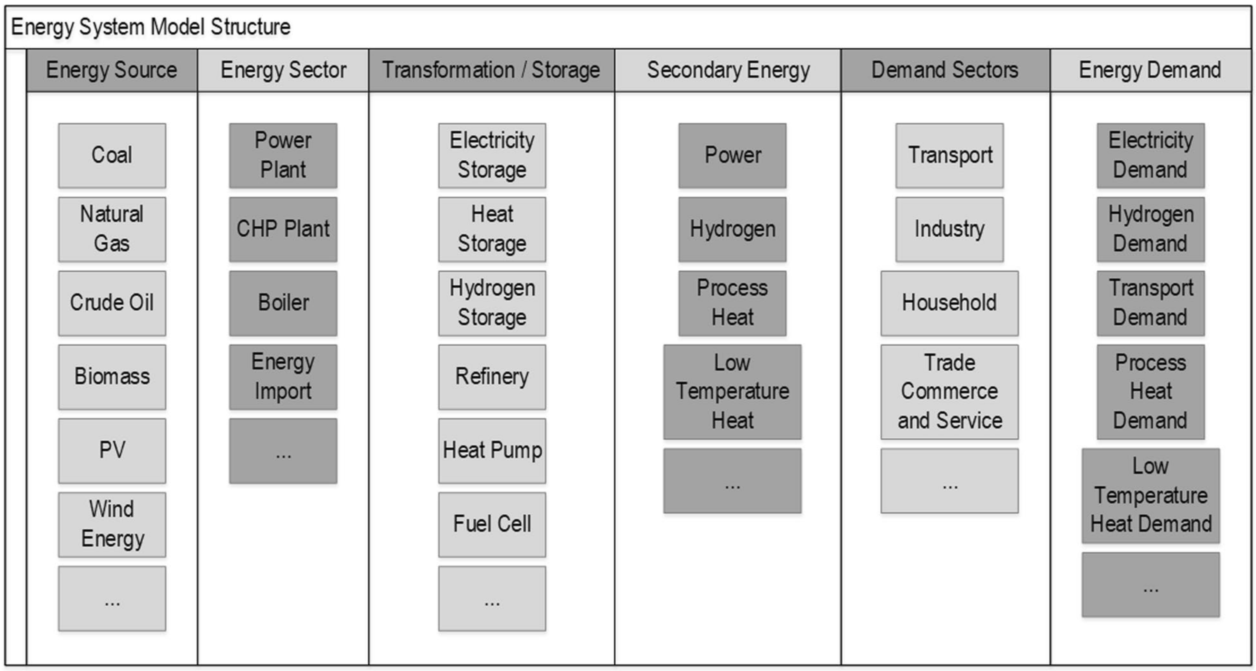

Fig. 7 Generic energy system model structure based on Wiese et al. [138]

Scope

This article assesses six widely used energy system models with a detailed industry sector, of which four models simulate future energy scenarios and two optimize future energy system design. The FORECAST model is used to develop future energy scenarios for long-term predictions of energy demand and GHG emissions. Therefore, it can be used as a strategic future decision support tool [131]. The focus of these simulations and their analyses is primarily Germany. The industry submodule embedded in the FORECAST module evaluates policy implications for the energy demand and GHG emissions of the total industry sector. Simulations are conducted at a very detailed technology level, down to sub-sectors like pulp and paper. The national energy modeling system (NEMS) is another simulation model that projects the energy production and demand of the future energy system in the US [134]. Based on economic, environmental and security of supply factors, NEMS addresses the impacts of various energy policies and assumptions about future energy market development. Initially, CIMS (Canadian integrated modeling system) [136] was used as the predecessor of NEMS, and only later developed further to completely focus on the Canadian market [132]. It simulates technological development, as well as energy production and demand in relation to developments in the Canadian market.

The energy system modeling environment (ESME) optimizes future energy system designs [133]. The system design and pathway leading to it are optimized on the basis of the minimal cost setup, which still satisfies all energy demands and remains within the constraints given. One goal of ESME is to analyze system designs without considering policies, which for example affect fuel costs. The TIMES integrated assessment model (TIAM) analyzes medium- or long-term planning strategies for future energy systems [137]. TIMES also optimizes the system design with respect to welfare maximization and the minimization of overall system costs. As with all of the mentioned energy system models, ETSAP-TIAM can generate exploratory energy scenarios and assess policy implications on energy system design [135].

Spatial and temporal extent

In light of the climate change mitigation targets of 2050, all of these energy system models can simulate or optimize an energy system design for that target year. However, bottom-up models in particular, which not only simulate the system design of the target year, but optimize the transformation path as well, will run into computation time problems when considering especially long periods. All six models have the capability to either simulate or optimize at an hourly resolution. FORECAST is a one-node model that focuses on energy system design and the transformation of Germany on a national scale. CIMS, ESME, NEMS and ETSAP-TIAM are multi-regional models and take commodity flows between regions into account. Meanwhile, ESME focuses on the United Kingdom, whereas NEMS was specifically developed to mimic the characteristics and technological development within the US market.

System boundary

The basic structure of an energy system model consists of the components for energy supply, energy transformation, energy storage and energy use (see Fig. 7). These components are connected via commodity flows, which state how much of what type of medium and which energy content flows from one component to another. Supply and demand can be satisfied by the conversion work of each component and their respective commodity flows. At all time steps, supply and demand must be constantly balanced in order to design a stable energy system.

All six energy system models consider the electricity, heat, transport and industry sectors to a certain degree, although the way in which these are modeled varies greatly. For the comparison of how detailed circular economy measures are implemented in each of these models, a closer look at the industrial sector follows. All analyzed energy system models model the industry sector in detail and disaggregate down to individual processes, except for ESME, which only accounts for the aggregated total energy balance within the industry sector. The NEMS model includes an industrial demand module, which covers 15 manufacturing and six non-manufacturing industries. The energy-intensive industries of aluminum, glass, iron and steel, as well as pulp and paper, are implemented in detailed individual process flows within submodules. This structure allows for the changing of the individual process technologies over time within one simulation run. The FORECAST simulation model covers more than 60 individual industrial processes and connected commodity and material flows, subdivided into four groups. Future projections of each process route in the FORECAST model are made based on exogenous drivers for demand development such as per capita demand or recycling rates. CIMS includes sub-models for chemical products, industrial minerals, iron and steel, metal smelting, metals and mineral mining, other manufacturing, pulp and paper, and petroleum refining. Within each sub-model, 38 (chemical products) to 243 (metal smelting) technologies compete to satisfy industrial demand with respect to the system constraints within a simulation run. The ESME model simulates the future energy demand of the industry sector by accounting for the energy demand of the individual sub-sectors, which are, however, not disaggregated down to the process level. Projections are made for each subsector with respect to the energy demand of that subsector in the base year 2010. Simulation of the industrial process behavior of industrial sub-sectors is not possible with ESME. The ETSAP-TIAM model, in contrast, can optimize the industry across 12 disaggregated sub-sectors, namely agriculture, food, metals, cement, other commodity production, wholesale, private service, public service, construction, other utilities and motor vehicles. In this way, modeling the actual material outputs from the industry sub-sectors is possible in ETSAP-TIAM. Individual processes can be optimized at a disaggregated level and subsequent implications for the total system can be analyzed. Of those models that have a detailed representation of individual process paths, the common bulk materials such as iron and steel, non-ferrous metals, as well as pulp and paper, are implemented in detail. More complex sub-sectors such as chemical processes are partly covered by FORECAST, CIMS, ESME and ETSAP-TIAM.

The analyzed models implement circular economy measures at varying levels of detail. The FORECAST model expends much effort to consider them as exogenous assumptions for their simulation runs. The ESME and CIMS in turn implement industrial processes in greater detail but neither considers material flows as such. Rather, both models rely on exogenous assumptions to consider measures such as material substitution. Although the NEMS and ETSAP-TIAM models consider material flows within industrial processes, the complete material cycle is not taken into account. The product output of the industry sector is not considered further in either energy system model, apart from satisfying the specific product demand, which drives production in the first place. The recycling of materials is based on exogenous assumptions and is implemented in the models as a reduced material demand over time. Consequently, apart from the costs for the recycling technology and process itself, no costs for the complete recycling path, including those for the collection, sorting and pre-treatment of waste, are considered. None of the energy system models considers a product lifetime, and so there is no way of determining when industrial output or energy conversion technologies become obsolete and could potentially return to the material cycle. Apart from waste use in energy conversion technologies, such as waste incineration plants, waste and end-of-life treatment of industry output or energy conversion technologies are not considered further in all of the analyzed energy system models. The FORECAST simulation model aims to include mitigation options based on material strategies, such as circular economy measures, recycling, material efficiency and material substitution. However, these options are considered through exogenous assumptions and are not implemented in the simulation model itself, and so must be defined in the scenario settings. The endogenous consideration of material cycles and their implications within the complete energy system have thus far not been part of any of the analyzed energy system models.

Underlying methodology

In general, energy system models are based on three different methodological approaches. Optimization models, such as ESME and ETSAP-TIAM, utilize linear, mixed-integer linear or non-linear programming techniques to solve objective functions to optimality [139]. It is assumed that one optimal solution exists, which could be a least-cost pathway for technology investments to reach a specific goal (e.g., CO_2 emissions reduction). How and to what extent the temporal boundaries for optimization of the objective function are set characterizes optimization models. A perfect foresight model, such as the ETSAP-TIAM, takes into account all possible future developments, such that over the entire time horizon the model can make certain decisions from the beginning on. Some models use a myopic approach and split the time horizon to consecutively optimize smaller periods and thus reduce the effect of previously made long-term assumptions [140]. The ESME attempts to minimize these future uncertainties by making use of stochastic approaches to determine the necessary assumptions. FORECAST, CIMS and NEMS are simulation models, which do not determine a single optimal solution but rather provide a variety of possible solutions, depending on how the input parameters (e.g., carbon tax price) have been set. Therefore, these models are also considered scenario-generating models, since not a single solution is discussed but several possibilities are compared and evaluated [141]. Apart from the differences in their solution space, optimization and simulation models differ in the way the user interacts with the model. Whereas for ESME and ETSAP-TIAM the user provides input data, objective function and restrictions to let the models determine the optimal solution, FORECAST, CIMS and NEMS are fed with potential system characteristics to compute a standard for decision-making based on the implications of various scenario input combinations.

The challenges of combining MFA and ESM

The following chapter illustrates how a successful combination of material cycles and energy system design can enable a more extensive analysis of energy system models, as well as the challenges that modelers of both material flow and energy system analysis must overcome.

Representation of industrial processes

The industrial sector combines material and energy flows and is thus crucial for coupling material flow and energy system models. According to Wiese and Baldini [142], energy system models must incorporate the industry sector in greater detail in order to analyze the impacts of sustainable industry routes on the entire energy system. Furthermore, Edelenbosch et al. [143] stress how the analysis of industrial sub-sectors in more detail improves the validity and robustness of the results. Although it appears to be scientific consent that a more detailed implemented industry sector is crucial for holistic analyses, it is still under debate which technologies and future measures should be assessed. A recent study by Davis et al. for example assessed how future net-zero emission energy systems should look like [144].They analyzed in detail how steel and cement production can become CO_2-neutral. In doing so, the study focuses on technology and fuel switches and is blind to potential measures of the circular economy. The authors conclude that on the one hand more research has to be done on potential processing technologies for difficult-to-decarbonize industries and on the other hand their cost-efficient systems integration must be analyzed as well (p. 7 [144]). A detailed and comprehensively modeled industry sector is the basis for the successful coupling of material flow and energy system models. The energy materials nexus and the energy-critical resources nexus are two major correlations which can be addressed by modeling industrial processes in greater detail. These correlations are admittedly the focus of the following two studies but the assessments are made in only one direction. McLellan et al. analyze mineral demand for future developments in the Asian region and assess potential resource criticalities, but not how producing or processing these minerals affects the energy system in return [145]. Di Dong et al. analyze copper production in China and how it reacts to the future energy transition [146]. They conclude that the energy transition can both decrease the environmental impact, due to changes of energy carriers and supply of low-carbon electricity, and increase the impacts due to a growing copper demand for innovative energy technologies and infrastructure. Furthermore, they state that recycling is beneficial for the environmental impacts of copper production but the feedback of subsequent changes in the energy system design was not examined. In order to depict the energy material nexus and analyze whether recycling is a cost-efficient climate gas mitigation strategy, certain process routes in the industry sector are of special interest to be modeled. To analyze for example fuel and technology switches in the production of steel, it is sufficient to model the conventional (e.g., blast furnace, basic oxygen furnace, etc.) and future innovative processes (e.g., H2 direct reduction) only. Once recycling measures are supposed to be part of the analysis, several more processes are needed. First of all, production techniques to process steel scrap with specific energy input and emissions output (e.g., electric arc furnace) are required. The waste management infrastructure for collection and preprocessing of steel scrap is equally important. Another crucial point is the estimation of future steel scrap availability. Therefore, the different fields of the use-phase of steel must be mapped within the model (e.g., construction, automobiles, machinery, etc.). With suitable methods and lifetime distributions (see for example [147]) it is possible to calculate the residence time of steel within these anthropogenic stocks and consequently know when steel scrap becomes available for the energy system again. This is especially important when not only a static energy system design in the future is to be analyzed, but also the transformation path in between. Depending on the system boundary and spatial context of the assessment, extraction processes (e.g., for iron ore) must also be considered. If the industry sector is implemented at a too aggregated degree, so that just the energy use of the entire sector or a sub-industry is considered, and no individual processes are modeled, CO_2 mitigation options specific to the industry cannot be assessed in the ESM [148]. As the majority of material flow models cover material flows and stocks within the two phases of manufacturing and production, energy system models must extend their industry representation to such a level of detail that material flows and stocks can be implemented, and so circular economy measures can be assessed. Pesonen [44] describes the same challenge in relation to coupling material flow models and economic data, and concludes that material flow models must be extended as well; material flow models must then cover well-known processes so that energy system models can implement them.

Aligning system boundaries

Differences in the system boundaries between energy system and material flow models pose a great challenge to successful coupling. The absence of sectors in one model that are covered by the other makes a comparable analysis difficult. An energy system model that does not consider a specific sector cannot account for energy flows related to the analyzed material flows and stocks in that sector and covered by the material flow model. This threatens the overall energy balance of the entire system. Classic material flow models aim to analyze the flows and stocks of a material over its entire lifecycle. An energy system model that wanted the inclusion of material flows and stocks had to depict all sectors where this specific material is present, even though some might be irrelevant for energy system analysis. According to Melo [149], the type of lifetime distribution has a substantial impact on the dynamics of material flows, especially scrap flows. Therefore, it is crucial that energy system and material flow models implement the same type of lifetime distribution for all relevant material data. Material flows usually have an international dimension which makes it difficult to cover all characteristics (e.g., extraction in one country and waste management in another country) in one national energy system models. The concept of the ecological backpack (a measure for hidden natural resources of a product or service [150]) could be applied to national energy system models to address the problem

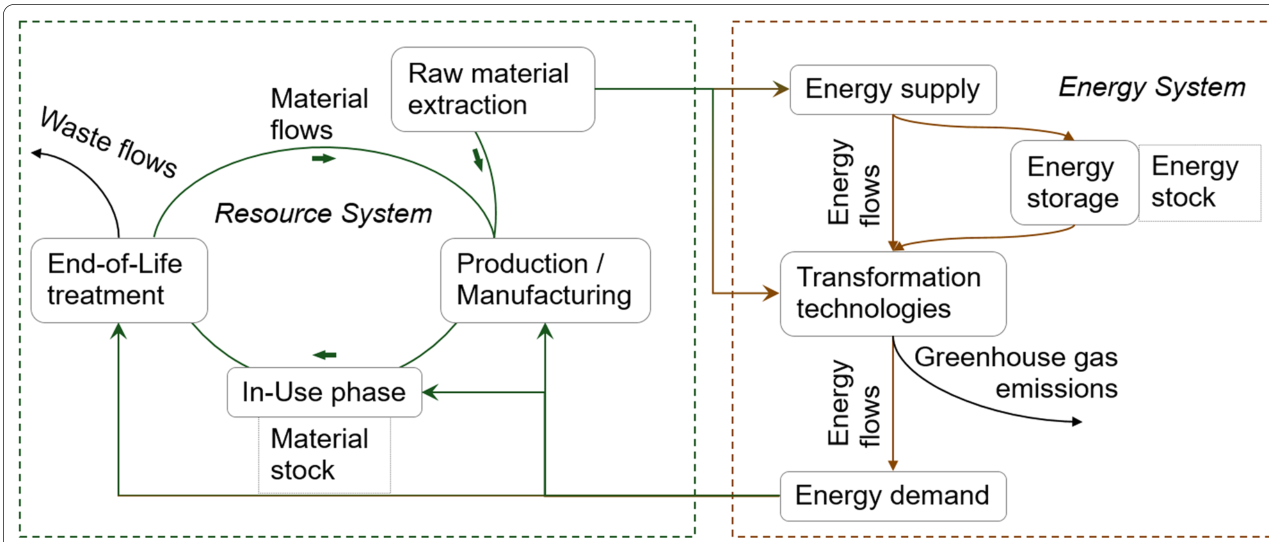

Fig. 8 *System boundaries of ESM and MFA; own illustration based on Velenturf* et al. [152]

of differing spatial extents, and to consider up- and downstream impacts of material flows and stocks. Before coupling material flow and energy system models, aligning system boundaries and ensuring that both models cover relevant sectors reduces the risk of missed material or energy flows. Not only does this lead to differences in system boundaries in terms of possible misses of important energy or material flows, but also, if system boundaries are aligned, energy and mass accounting problems can occur through double-counting. The risk of double-counting when coupling energy system and material flow models is particularly high for those material flows that are simultaneously energy flows. As an example, material flow models could analyze the lifecycle of wood as a construction material, and at the same time, energy system models could analyze wood as an energy carrier. A coupled model must then analyze which fraction of a material flow is energetic and which is purely material and subsequently analyze the related material and energy flows within the total coupled system (see Fig. 8). Wider system boundaries diversify the transformation pathway to low-carbon energy systems and add to the achievement of additional sustainability goals [151].

Each model can benefit from inputs of the other and increase its relevance and robustness

As stated by Binder (2007) [43], the results of material flow models are too seldom the basis for policymakers. The results of models that focus on a single, or a few categories, such as material flows, can analyze that specific category in detail, but the overall system is beyond the scope and interactions with other categories are left unaddressed or analyzed. Policy recommendations resulting from these models might work in opposite directions, which makes it difficult for decision-makers to enforce the optimal policy. Energy system models, which analyze energy system design, yield investment recommendations for energy conversion technologies. Material flow models, on the other hand, analyze material cycles and yield policy recommendations, aimed at increased waste collection or improved recycling rates. The impacts of how higher recycling rates resulting from policy recommendations derived from material flow models influence future investment decisions, which result from policies originating from energy system analysis, cannot be foreseen. Combining those two models will result in more sound results and policy implications and, thereby, in greater political significance for both energy system design and material cycles.

Which underlying methodology?

With the increasing availability of better computing resources, a trend from solely simulation models towards more complex optimization models in energy system modeling can be observed [48]. Together with the insights of O'Brien [153], who found that optimization models are more suited for quantitative analysis, whereas simulation models are rather used for qualitative assessments, energy system modeling will tend to answer more quantitative rather than qualitative research questions in the future. This is in line with the basic concept of MFAs to quantitatively assess material flows and stocks in society, and thus a suitable interface for a combined ESM and MFA. More problematic is to combine static or solely retrospective MFAs with ESMs. Static MFAs can only serve as data input for ESMs, which optimize or simulate a single point in time rather than a transformational pathway analysis. Retrospective MFAs provide no real benefit for ESMs, which analyze future energy system designs. In general, the underlying methodology is not a decisive factor for whether a coupling of ESMs and MFAs is successful or not. Rather, differences in methodology are merely an indicator of how data are structured, in which format data are available and how it can be used as input for ESMs. In addition, scenarios of future material use are far less represented in literature than accounting of historic material flows and stock. However, these estimations of future material flows are crucial for analyzing their effects on prospective energy system designs [154].

Which data are needed?

Material flow models require flow and stock data of the material under investigation within the system boundary. As the outputs of material flow processes are complex products, the ratios of material concentrations in all relevant products are also crucial. In order to limit the amount of data that must be handled, material flow models must preselect which material flows and processes should be included in the main analysis. Preselection is based on guidelines that state that only material flows, which make up more than 1% of the largest flow, should be included in the material flow analysis [14]. Important to note is that the guideline refers to both the quantity of a flow as well as its material concentration. Flows that make up less than 1% of the largest flow might still be of importance due to the high concentration of the material under investigation. Pesonen [155] stresses the importance of ranking all flows, which will be affected by model coupling and by their significance in the individual model. Following this, there are flows that are important for both, only one or none of the coupled models. As an example, one important process flow for both the energy system and material flow models is waste incineration. Large material flows enter waste management processes, which makes them interesting for material flow analysis, and large energy flows result from waste incineration, which stresses the impact on the energy system design and the importance of including it in energy system models. Any waste resulting from an energy conversion process is of little interest for energy system modeling. However, especially if this waste causes environmental stress, material flow models deem such flows and stocks important. Quantitative and qualitative information on energy flows between conversion technologies are therefore necessary. A combination of material flow and energy system models requires this specific information for flows and processes. Flows and processes are then aligned to result in a single process and flow, which still holds all of the information for both models. Therefore, data must be on the same temporal and spatial scale and cover the same system boundary. Additionally, data availability varies greatly with the spatial scale for different model types [49]. Data at the regional or local scale is more difficult to acquire compared to that on a national scale. Not only do both energy system and material flow models need to be at the same spatial scale, but the spatial scale itself threatens data availability. A disaggregation or aggregation of data could therefore become necessary in order to successfully combine material flow and energy system models.

Another issue that exacerbates the nexus of material and energy flows is the transparency and openness of material flow and energy system models, as well as their data. According to Binder et al. [43], it is problematic to acquire the necessary data for a comprehensive material flow analysis, and additionally, data uncertainty threatens the significance and reliability of the results. Most of the reviewed material flow models provide some supplementary data together with their publication. The framework itself is admittedly seldom publicly available, but due to their mostly straightforward underlying methodology of material flow and stock accounting a minor obstacle. Even though Lopion et al. [48] found a trend in energy systems analysis towards more open-source development (see for example OSeMOSYS [156] FINE [157], Calliope [158], oemof [159] or PyPSA [160]). However, open-source modeling implies the model structure and code only and not the data for parametrizing. Data used in energy system models is usually not publicly available. However, a study by Morrison [161] sees increasing efforts in the open-source development of energy system models and also their corresponding datasets. The lack of publicly available data is a threat to any transparent approach to combine material flow and energy system analysis. Being able to answer a greater variety of research questions, while holistically analyzing energy systems, and also gaining public acceptance, demands an open-source energy system model with transparent use of publicly available material flow data.

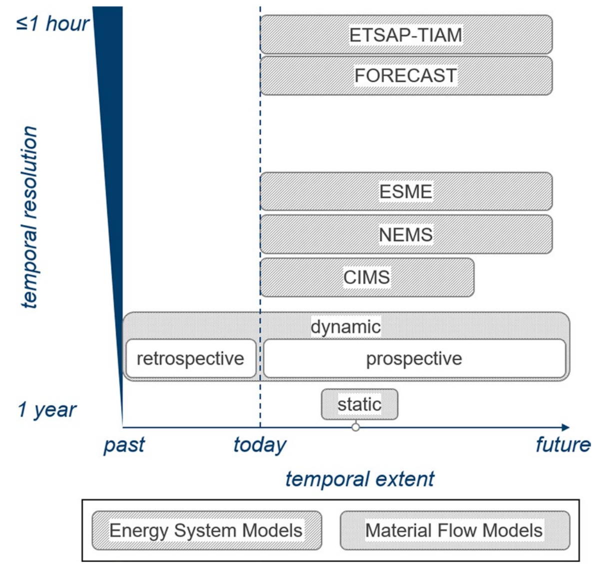

Fig. 9 Classification of MFAs and reviewed ESMs by temporal resolution and extent

Temporal resolution

The temporal resolution describes how detailed considered periods are broken down and modeled. Lopion et al. [48] found that the trend in energy system modeling tends towards higher resolved and thus more complex models due to the availability of high-performance computing resources. NEMS and ESME represent one year through several time slices and seasons. A sufficiently high temporal resolution is a decisive factor, whether certain research questions can be answered by the model. For example, a yearly representation of 8760 h, as in the ETSAP-TIAM model, allows for highly fluctuating renewable energy technologies to be analyzed as well. MFAs do not require such a high temporal resolution to answer research questions specific to the material flow community. All of the reviewed MFA models exclusively use a yearly resolution. Comparing the requirements for temporal resolution elucidates yet another conflict between both modeling communities (see Fig. 9). The implementation of material flows into the ESMs either binds the temporal resolution of the ESM to one year or the flow and stock data of the MFA must be temporally disaggregated to the desired level of resolution. Whereas the first approach is relatively simple to implement, the resulting ESM is no longer able to answer research questions aimed at higher levels of temporal resolution. The second approach maintains the temporal flexibility of the ESM but requires disaggregation work in advance of the coupling. Acquiring the material flow data with a temporal resolution of 365 days or 8760 h is a difficult task, as official statistics only report country-specific data on a yearly basis [162]. In addition to the temporal resolution, the temporal horizon can limit the combined analyses of material and energy flows. Material flow models must be able to estimate future material flows and stocks to give meaningful input for energy system models. For some materials these future flow and stock developments exist (see Watari et al. [151]) which allows for implementation in energy system models.

Conclusion

The transformation of a fossil-based energy system towards a low-carbon one is inevitably linked to a shift in resource use and raw material availability. This link is a two-way connection. Not only do new low-carbon energy technologies affect raw material use, but resource use also has an influence on the energy system's design. The concept of the circular economy describes the utilization of material in societal cycles so as to minimize related environmental impacts. This review shows that the influence of the cyclic use of material on the energy system can currently not be assessed with state-of-the-art energy system or material flow models.

Material flow models can assess circular economy measures and evaluate recycling policies or material efficiency strategies. These models, however, do not consider the entire energy system, or cover only individual energy flows, and so a holistic assessment of material and energy flow interaction is impossible. Energy system models implement energy flows at a detailed level but currently leave out material flows and stocks within the energy system. Currently, the development of material flow models runs parallel to the one of energy system models. Both communities would benefit from a combined progression.

For a successful combined approach of material flow and energy system analysis modifications in the following categories have to be made.

Representation of industrial processes

As the industrial sector accounts for an important share of national material flows, it must be modeled in sufficient detail. Industrial energy demand, which is assumed in most energy system models on an energy balance level only and not linked to material flows, does not provide an adequate basis for implementing circular economy measures. To evaluate recycling measures based on effectiveness and cost-efficiency as a climate gas mitigation option, the industry sector implementation must include processes within the lifecycle phases of production and manufacturing of industrial goods, and a depiction of the anthropogenic stock and waste management to assess when material becomes available for the energy system again. Depending on research question and system boundary, especially in light of growing demand for critical materials, the consideration of the life cycle phase of raw material extraction becomes important as well.

Aligning system boundaries

Coupling models always carries the risk of describing the same phenomenon in each model and thus double-counting it. This problem arises, for example, when differentiating between the energetic and material share of material flows in the coupled system. Being aware of the different accounting boundaries is important to reduce the risk of missed energy or material flows. It is therefore crucial to align system boundaries and ensure that both models cover relevant sectors. This specifically applies to the spatial extent of national energy system model. Since material flows, critical resources in particular, have an international dimension (in most cases even global), the assessment is limited to the impacts within national borders. For a complete picture of the energy material nexus, national energy system models must consider upstream effects of material import and downstream effects of material export, by incorporating an ecological backpack.

Methodology

Every material flow model is based on balancing input flows, stocks and output flows either static, that is for one specific point in time, or dynamically over a certain period. The underlying methodology is not based on optimization or simulation like in energy system models. Static MFAs can serve as data input for ESMs, which optimize or simulate a single point in time. ESMs, which analyze the future energy system design over a transformation path require data input from a dynamic and prospective MFA. These MFAs perform estimations of future material flows and stocks under exogenous assumptions. Through the coupling of material and energy flow analysis certain assumptions become endogenous, for example the development of future copper demand through expansion of photovoltaic is then determined by the internal energy system analysis, while others remain exogenous, for example the demographic development.

Data

Quantitative and qualitative information on energy and material flows within the energy system are necessary. Unfortunately, data availability varies greatly with the spatial scale for different model types. Material flow data are more difficult to acquire, especially at the regional and local scale compared to data on a national scale. Additionally, accessibility to material flow data is often limited. The lack of publicly available data is a threat to any transparent approach to combine material flow and energy system analysis. Whereas the trend of material flow and energy system model development is towards open-source software, the underlying datasets are seldom published. Open and easily accessible datasets make a holistic analysis of the energy material nexus possible in the first place, and enable scientific reproducibility in the long run.

Temporal resolution and horizon

Most commonly, material flow and stock data are available as a yearly value that has to be introduced into energy system models, which mostly work on a more disaggregated temporal resolution (often ≤ hourly for integration of fluctuating renewable energy sources). Yearly material flow data can be implemented as hourly averages, for instance. More importantly, a material flow model must be able to project material flows and stocks from today into the future. Energy system models can then use these material supply and demand data for the analysis and dimensioning of the future energy system design. The temporal horizons of the projected material flows and the energy system design have to be the same.

Each model can benefit from inputs of the other and increase its relevance for decision-makers

A coupled model via either soft- or hard-coupling enables more robust and significant results, a reply to a greater variety of research questions and comprehensible analyses. Furthermore, the energy system analysis and material flow analysis community will benefit from this, as a coupled model would stress the interactions of material and energy flows, result in more robust energy system scenarios and thus make combined implications more relevant for policymaking. A joined energy and resource picture can expose significant potential flaws that remain unrecognized by an individual assessment, which can lead to improved decision-making.

It is important for the energy system research community not to only create energy scenarios, but also provide a depiction of resource use and demand along with it. The circular economy principle has become a major part of political strategies and therefore models must be able to combine the objectives of both the energy and resource sectors.

This paper indicates the need for more cohesive and interdisciplinary approaches resulting from collaborative models of the energy system and material analysis research communities. These models must remain easy to use and intuitive, even after coupling. Models that predict or optimize pathways to a future sustainable and cost-efficient energy system design, which meets climate mitigation targets, must consider anthropogenic material flows and stocks in order to guarantee a comprehensive knowledge base for decision-making.

Finally, for society to accept and take on the challenges associated with the energy transition, energy system analyses must be considered from many different angles including circular economy measures, such as recycling.

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