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Energy systems modeling and optimization for absolute environmental sustainability: current landscape and opportunities

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ABSTRACT

Energy systems analysis supports in designing and operating reliable and cost-effective energy solutions to a range of sectors, including power, heating, mobility, and industry. Notwithstanding the wellbeing and prosperity implications for current generations, it becomes increasingly clear that our current global energy system has profound impacts on our planet, potentially breaching the safe operating space for humanity. Life cycle assessments are broadly used to account for environmental aspects, however, this traditional approach may fall short of designing truly sustainable alternatives. Here, we review the concept of absolute sustainability and how it can be incorporated into energy systems modeling and optimization. Besides providing background, guidance, and perspective, we also discuss some challenges related to environmental and computational aspects. Although much work is still required, the absolute environmental sustainability concept can already be used in energy systems modeling and would contribute to achieving a green energy transition within planetary boundaries, ensuring sustainable development for future generations.

1. Introduction to absolute sustainability in energy systems modeling

Energy is the lifeblood of human civilization; it provides light in the dark, keeps people warm in winter and cool in summer, powers chore-easing appliances, greatly reduces the time needed to transport people and goods between locations, and fuels the processes and activities that produce everything we consume as a society. The systems that supply energy in its various forms are highly complex and deeply integrated with the human-built environment (Bale et al., 2015). They include several generation and conversion pathways from fossil and renewable resources with different characteristics, vast networks of transport, distribution and final use infrastructure, and sophisticated market and non-market arrangements to match ever-changing and fluctuating supply and demand.

Notwithstanding the enormous benefits energy systems have brought to humankind, their current environmental impacts exceed our planet's carrying capacity and their damage to human health can be considered unacceptable. For example, energy use is responsible for over 70% of global greenhouse gas (GHG) emissions (Ritchie and Roser, 2020) and millions of deaths are attributed to airborne particulate matter from fossil fuel combustion (Vohra et al., 2021). Recent and upcoming technologies in energy generation (e.g. solar photovoltaic and wind turbines), energy storage (e.g. Li-ion batteries, power-to-gas), alternative energy carriers (e.g. green hydrogen and methanol) and energy demand management (e.g. smart grids) promise more environmentally benign energy provision (Davis et al., 2018). Nevertheless, adapting existing energy systems is difficult due to their technical

Abbreviations: AESA, Absolute environmental sustainability assessment; ESM, Energy systems models; GDP, Gross domestic product; GHG, Greenhouse gas; GVA, Gross value added; IAM, Integrated assessment models; LCA, Life cycle assessment; LCI, Life cycle inventory; LCO, Life cycle optimization; LP, Linear programming; MILP, Mixed integer linear programming; MINLP, Mixed integer non-linear programming; MOO, Multi objective optimization; PB, Planetary boundary; PDF, Probability density function.

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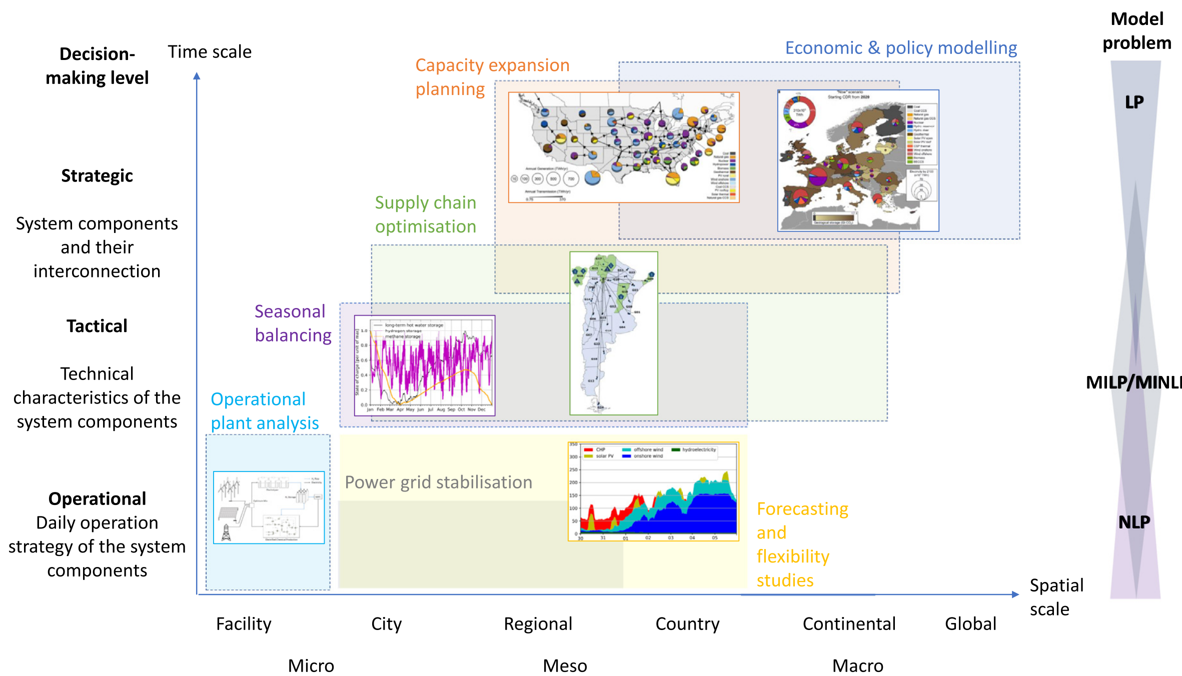

Fig. 1. Multi-scale modeling for energy systems in the process systems engineers community. Adapted from (Brown et al., 2018; Galán-Martín et al., 2018; Galán-Martín et al., 2021; Wheeler et al., 2021).

complexity, their criticality to human life and political stability, their interconnectedness with multiple industries and sometimes competing interests between industries and communities (Cherp et al., 2011). Further, decision- and policy-making for energy not only need to consolidate economic and environmental factors but also multiple potential trade-offs between environmental impacts (Luderer et al., 2019). Thus, the design of holistically sustainable energy systems is of critical importance to the flourishing of the human race throughout the next centuries.

Of interest to the modeling community, which works on designing and improving such systems, are multiple scales, from micro to macro, and the associated applications (Fig. 1). For example, on the macro scale, we study energy use within the whole economy (McCollum et al., 2018; Pehl et al., 2017), as well as continent-wide or multi-region power systems (Galán-Martín et al., 2018; Tröndle et al., 2020). On the meso scale, we assess regional multi-sector energy systems (Baumgärtner et al., 2021) or optimize regional fuel supply chains (De-León Almaraz et al., 2014; Ehrenstein et al., 2020). On the micro scale, we investigate the interplay between local generation and single demand sites (Chen and Yang, 2021; Martín and Grossmann, 2017) or determine the ideal energy provision according to local land availability (Leung Pah Hang et al., 2016; Calvert and Mabee, 2015).

The quest for sustainable energy includes designing and optimizing energy technologies and systems considering multiple criteria beyond economics, i.e., incorporating environmental and socio-political concerns at the core of the decision-making process. Today's prevalent approach to assess the sustainability level of industrial systems, including energy systems, is based on life cycle assessment (LCA) methodologies, which were recently combined with optimization models (Volkart et al., 2018) following the life cycle optimization (LCO) framework. LCA emerged through collaboration between industry and academia as a method for gauging the environmental performance of industrial products, services and technologies (Azapagic, 1999). LCA has later been adopted in many fields to quantify and compare the environmental impacts of technologies, products or services across their full life cycle (e.g. mining, logistics, processing, use, maintenance, end-of-life disposal of solar panels) and across multiple damage categories to comprehensively express impacts on the environment, human health and resources (Bjørn et al., 2018). Hereby, LCA allows for approximating well the real and multifaceted impacts from e.g. energy systems (Laurent et al., 2018). Critical in the assessment of energy systems, LCAs shed light on more than just GHG emissions, thus revealing potential unexpected trade-offs, i.e. shifting the burden from one impact category to another (Algunaibet and Guillén-Gosálbez, 2019; Negri et al., 2021a), but also welcome co-benefits, i.e. reducing burdens in multiple impact categories simultaneously (Volkart et al., 2017).

However, LCAs have several shortcomings when used to support political and business-level decisions. First, LCA studies commonly provide results for 15+ different metrics where many can be difficult to interpret for non-experts. This can lead decision-makers to focus on the easier-to-understand indicators (such as climate change) (Freidberg, 2015). The problem is exacerbated by the fact that trade-offs often arise in the design and operation of energy systems, which makes the interpretation of the results more challenging. One approach to address this problem has been through the monetization of impacts. This method internalizes external costs to society (e.g. through remediation, lost opportunities or health expenditure), incorporating the environmental and human health aspect as costs into the economic bottom line (Algunaibet et al., 2019a; Freire Ordóñez et al., 2021). However, monetization of impacts is controversial as the scientific base to estimate the cost is problematic at best since it is a) challenging to determine the contribution of certain emissions to causes and events (van Oldenborgh et al., 2021) and b) accurately capture the loss and damages across the globe (Clarke et al., 2021; James et al., 2014). These factors might lead to a significant underestimation of total societal costs due to nonlinear events (Stern, 2013).

Second, and connected to the previous point, to enable interpretation across LCA metrics, normalization is often done where impacts of the studied activity are related to a reference. The reference can be in the form of other similar activities or the impacts of human society in the respective impact categories. This can be considered as a relative sustainability assessment because the performance of the studied activity becomes relative to the selected reference (Ryberg et al., 2018a), while it completely disregards geophysical and biological limitations, i.e. whether global, regional, or local biospheres can absorb those impacts (Bakshi et al., 2018). Thus, normalization using an anthropogenic reference is blind to the fact that, in some impact categories, humankind already operates in heavily unsustainable ways, such as climate change and biodiversity (Pörtner et al., 2021).

A novel promising approach to perform environmental assessments (appealing from a scientific and communications perspective) is based on the concept of absolute environmental sustainability (Hauschild et al., 2020), which takes into account the carrying capacity of our planet or, in other words, the planetary boundaries (PB). The basis of the concept is that the Earth's climate and conditions have been relatively stable for the last 10,000 years (i.e. the Holocene) and enabled human societies to thrive. However, the Earth system's ability to absorb human-caused impacts and stay within these conditions is limited (Rockström et al., 2009). A loss of stable conditions and Earth system resilience is most likely less conducive for human life and might severely compromise the well-being of future generations. The approximation of those limits for different impact categories and what they imply for delineating a "safe operating space" (SOS, where the risk of destabilization is kept low), is the subject of the science of planetary boundaries. The last decade has witnessed a plethora of new research, not just in further understanding Earth system processes (Wagener and Pianosi, 2019) but also in quantifying the SOS to guide human development (Steffen et al., 2015). This new field of study provides ceiling indicators for anthropogenic impact, identifying truly sustainable options, lifestyles, and practices. Consequently, an increasing number of studies using some form of absolute sustainability have been carried out (Bjørn et al., 2020).

The paradigm shift from relative to absolute sustainability in LCA was accomplished by linking the LCA methodology with the PB framework (LCA-PB) through characterization factors of impact pathways (Bjørn and Hauschild, 2015; Ryberg et al., 2018b; Ryberg et al., 2021). These emerging absolute environmental sustainability assessments (AESA) methods allow evaluating the absolute sustainability level of industrial systems, including energy systems, by using them in combination with standard mathematical approaches such as optimization and scenario analysis. The planetary boundaries can also be downscaled to the level of the studied activity in different ways (Ryberg et al., 2020), allowing to define impact reduction targets for individual projects, corporations or countries (Sandin et al., 2015). Applying these novel concepts together can help with the tremendous task of holistically redesigning our global, regional and local energy systems (Khan, 2019), ensuring long-term sustainability and viability while minimizing unintended consequences (Bjørn et al., 2020). So far, however, planetary boundaries studies of energy systems are scarce (Bjørn et al., 2020) and global energy systems models (ESM) either completely omit sustainability criteria (Child et al., 2018), include LCA but are limited to climate mitigation (Baumgärtner et al., 2021; Brown et al., 2018; Zhu et al., 2019), or quantify multiple impact categories but not relative to the geophysical boundaries (Cheng et al., 2017).

To aid in the design of sustainable energy systems, this paper reviews the main advances in absolute sustainability assessments and provides guidelines on implementing them in this field. We also discuss the main methodological challenges of the AESA methods as applied to energy systems. Finally, we highlight further practical and computational challenges scientists and practitioners might face in this field. We conclude by outlining some future research directions.

2. Concepts of energy systems exploration for absolute sustainability

2.1. Energy systems modeling

The modeling of energy systems has an almost 50-year tradition, where at first techno-economic models were developed in the wake of the oil crisis in 1973 (Herbst et al., 2012). The nature of models is usually exploratory, relying on approximations and simplifications of reality to simulate policy, technology, and investment choices. Initially, different practitioners tried to address questions around energy according to their discipline. These include economists with top-down macroeconomic models (input-output, econometric or general equilibrium models) and engineers and scientists with bottom-up process-oriented models (optimization or simulation models).

Macroeconomic models are used to understand the impact of policies, such as CO_2 prices or subsidies, on the economy (including labour, capital and trade) but only consider final energy use and are typically unable to model structural change, technological progress, and smaller scales (Subramanian et al., 2018).

Process-oriented models are technology-rich and explicitly simulate possible arrangements for energy supply based on business economics (e.g. using capital costs and interest rates) but tend to exclude any consideration of market forces (Crespo del Granado et al., 2018). Here, we find a wide range of models addressing various problems, from supply chain planning to the design of power facilities, utility systems and microgrids, spanning multiple temporal and spatial scales. For example, at the process level, heat integration has received much attention (Klemeš and Kravanja, 2013) and its natural extension to embrace the design of utility systems (Andiappan, 2017). More recently, models integrating chemical processes with renewable sources have attracted increasing interest (Schiffer and Manthiram, 2017). This trend has been primarily motivated by the emergence of carbon capture and utilization routes based on electrolytic hydrogen, which requires vast amounts of energy (Rambhujun et al., 2020). At a larger scale, ESM were also introduced to optimize the portfolio of power technologies that could cover the energy demand reliably (Subramanian et al., 2018). Such models were also adapted to address the design of microgrids at a lower spatial scale (Fathima and Palanizamy, 2015). Other models focused on power distribution and electricity markets (Cali et al., 2021), optimizing prices and the power flow.

Nowadays, soft and hard-linked integrated assessment models (IAM) with a focus on energy systems combine elements of both approaches. Notably, IAM couple simplified climate science and economic models with models of energy system technologies to evaluate different economic, population and technological pathways consistent with given climate change mitigation targets (Hare et al., 2018). A range of IAM have been developed to aid with international climate negotiations and define shared socioeconomic pathways (Riahi et al., 2017), including IMAGE (Stehfest et al., 2014), TIMES (Loulou and Labriet, 2007), REMIND (Luderer et al., 2015), MESSAGE (Huppmann et al., 2019) and POLES (Keramidas et al., 2017). Other ESM have included macroeconomic developments as exogenous parameters and focus more on user-friendliness and open-source software, most notably OSeMOSYS (Howells et al., 2011) and Py-PSA (Brown et al., 2018).

The ultimate goal of the ESM defines its features, e.g. time step, temporal horizon, spatial resolution, and modeling approach. The goals can be a) strategic, e.g. in policy analysis or long-term investment decisions, where system components and their interconnection are defined, b) tactical, e.g. in capacity allocation and short-term investment decisions, or c) operational, e.g. in scheduling and grid balancing, where daily strategies of system components are defined (Fig. 1). To accomplish these goals, ESM either portrait a snapshot in time (e.g. a reference year) in a hypothetical future or build on existing infrastructure and develop least-cost or least-impact pathways to a desired state in the future (a capacity or generation expansion problem). For the latter, models are further differentiated by the foresight approach; in perfect foresight, complete knowledge across the study period is assumed, thus optimizing for the whole period simultaneously. In myopic foresight or rolling horizons, investment decisions are made sequentially, assuming only knowledge about the current period is available (Babrowski et al., 2014). This reduces model complexity and reflects industrial reality but might lead to a sub-optimal selection of technologies (Thomsen et al., 2021). Further review and classifications of existing ESM can be found elsewhere (Hall and Buckley, 2016; Ringkjøb et al., 2018).

2.2. Mathematical modeling and optimization

In what follows, we shall consider general ESM approaches optimizing strategic, tactical or operational decisions at different temporal and spatial scales. Many modeling tools have been applied to study energy systems, including simulation-based models, partial equilibrium models (Herbst et al., 2012) and agent-based models (Huckebrink and Bertsch, 2021). Notwithstanding these approaches, we here focus on optimization-based models based on mathematical programming tools. Accordingly, we shall consider the standard mathematical formulation for optimization problems:

$$\min_{x,y} \{\psi_k(x,y)\}$$

$$s.t. \quad h(x,y) = 0$$

$$g(x,y) \leq 0$$

$$x \in R^n, y \in \{0,1\}$$

where $\psi_k(x,y)$ denotes the different objective functions indexed by the subscript k, which can be economic, environmental or societal, x and y are continuous and binary variables, and $h(x,y)$ and $g(x,y)$ describe equality and inequality constraints that impose limits on the variables. Here, continuous variables often model technology capacities and mass and energy flows, while integer ones represent the system's topology, e.g. technology choices.

The model can take the form of a linear (LP), mixed-integer linear (MILP), nonlinear (NLP), or mixed integer nonlinear programming (MINLP) problem, depending on the nature of the objective function(s) and constraints. Integers and non-linearities increase the complexity of the model and thus the computational time and requirements. Different types of non-linearities can be encountered in practice, which often lead to nonconvexities resulting in multi-modality (i.e. multiple local solutions). Hence, different applications have different requirements. Process models often lead to nonlinear formulations due to the nature of the unit operations that are simulated in detail, which requires nonlinear mechanistic equations, including thermodynamic correlations. Conversely, increasing the scale often leads to simplified models that apply linear representations of the technologies modeled. For instance, turbines might be modeled with nonlinear formulations at the process level, while they might be simplified and approximated with linear capacity constraints and fixed yields in a supply chain or macro-economic model. Moreover, supply chain models with multiple possible connections, e.g. those introduced for bioethanol (Wheeler et al., 2021) or hydrogen (Ogumerem et al., 2019; Ehrenstein et al., 2020) as energy carriers for the transport sector, typically require integer variables. In contrast, large-scale power systems (Algunaibet et al., 2019b; Galán-Martín et al., 2018) and sector interactions (Baumgärtner et al., 2021; Brown et al., 2018) are often modeled with simple linear programming (LP) formulations. Such LP formulations greatly reduce the CPU time compared to an MILP model; the REMix Expansion model, for example, has 488 nodes and 8760 time steps per year with over 43 million variables and 32 million constraints (Scholz et al., 2020), which would be challenging to solve with an MILP or MINLP formulation.

An overview of potential input data to an optimization model is shown in Fig. 2. Data include technology and life cycle inventories, typically sourced from databases and literature; aggregated or spatially-explicit renewable energy resource availability and demand profiles, which can be sourced from bespoke datasets or Geographical Information Systems software; and projections related to capacities and demand drivers. An economic objective function typically includes capital expenditure, the weighted average cost of capital, fixed operating expenditure and the cost of consumables, e.g. fuel. The environmental objective function shall be described later in this article.

Mathematical programming has greatly evolved in the last decades, enabling the solution of previously intractable problems. Open-source software (e.g. Python) and solvers (e.g. GLPK, CBC, Ipopt) are available to the community, but commercial modelling software (e.g. GAMS (Bussieck and Meeraus, 2004), AIMSS (Bisschop and Entriken, 1993) and AMPL (Fourer et al., 2003)) and solvers (e.g. Gurobi (Gurobi Optimization, 2021), CPLEX (IBM, 2017), Xpress (FICO, 2018)) can often handle problems more effectively, particularly when dealing with nonlinear formulations (Anand et al., 2017), and are used in the most eminent models.

2.3. Life cycle assessment methodology to quantify absolute sustainability

For an energy system to be deployed in practice, it should be not only economically appealing but also environmentally friendly. Evaluating the environmental performance of energy systems requires performing a detailed LCA covering all their life cycle stages. This section explains relevant LCA concepts and provides a basis for implementing absolute sustainability into optimization models.

Energy systems consist of physical infrastructure, e.g. a wind turbine or a coal power plant, and require material inputs to operate, e.g. fuel or water. Multiple stages in the life cycle of infrastructure (material extraction, construction, operation, decommissioning) and inputs such as fuel (extraction, processing, distribution, combustion, residue disposal) entail diverse burdens to the environment that need to be quantified precisely to gain a full understanding of the environmental performance of energy systems (Laurent et al., 2018). Assessing the sustainability level of energy systems and consistently accounting for all those impacts in a practical way requires employing sound and comparable methods. This is typically realized by following LCA standards (e.g. ISO14040 (ISO, 2006)) and resorting to life cycle inventory (LCI) databases (Hammond et al., 2015).

According to ISO 14040, an LCA study consists of four steps (1) Goal and scope definition, (2) Inventory analysis, (3) Impact assessment and (4) interpretation, with details found elsewhere (e.g., Rebitzer et al., 2004). In step one of the LCA, the goal of the study, the functional unit (e.g. X kWh of regional electricity demand met) and the system boundaries need to be defined. The LCI phase, step 2, gathers the necessary data on feedstock requirements, emissions and waste to carry out the impact calculations (see Fig. 3). A standard LCA distinguishes between the foreground and background systems. The former represents the main activities over which we have a certain level of control, e.g., a coal plant whose carbon footprint one wishes to quantify. The latter includes all the processes

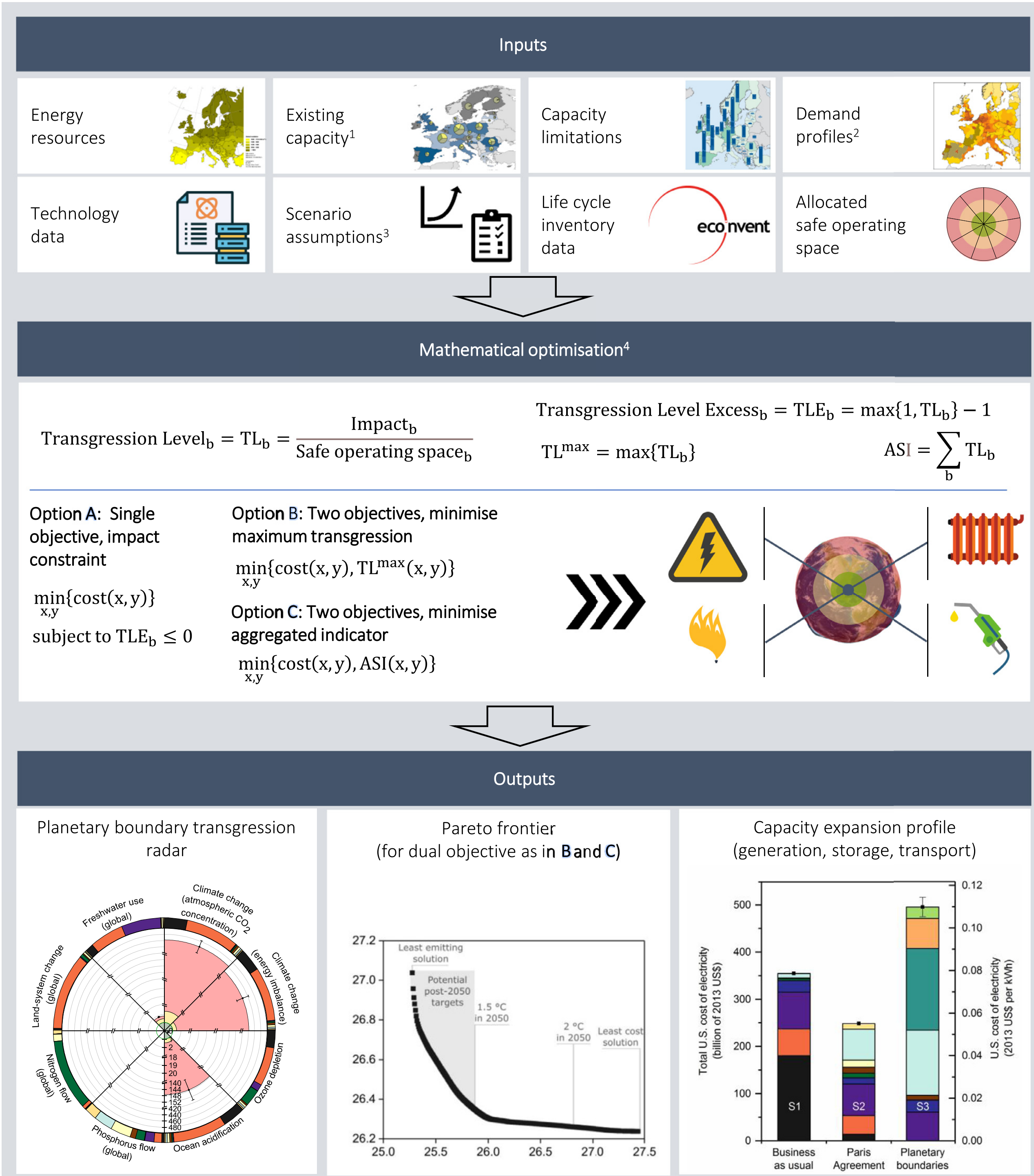

Fig. 2. Methodology overview of an absolute sustainability LCA study for ESM. 1 Generation, transmission, distribution and conversion infrastructure, 2 Power, heat, transport, 3 E.g. Reliability constraints, technology deployment rates, 4 Suffix b stands for the absolute sustainability impact categories (e.g. the nine planetary boundaries). Figures from (Energie-Atlas GmbH, 2005; CGN2010, 2015; Algunaibet et al., 2019b; Algunaibet and Guillén-Gosálbez, 2019; Komusanac et al., 2020; Negri et al., 2021).

in the supply chain connected to the foreground system, e.g., coal extraction, steel generation, etc.

There are several approaches to combine LCA with ESM, most notably post-processing and direct incorporation into the model (Laurent et al., 2018). The post-processing approach entails (arguably) a weak integration between LCA and ESM, where extracted results data from existing ESM – always including at least infrastructure (e.g. deployed capacity) and fuel use – are entered into LCA software, such as Simapro, openLCA, or Brightway with more software options listed in Pieragostini et al. (2012). In this case, the scope is predefined by the structure of the existing ESM (Tonini and Astrup, 2012). Hence, following this approach, the life cycle inventory is based on the simulation outcome, which is combined with data from environmental databases, often through the implementation in an LCA software package (Hammond et al., 2015). Here, impacts are merely assessed for the cost-optimal so-

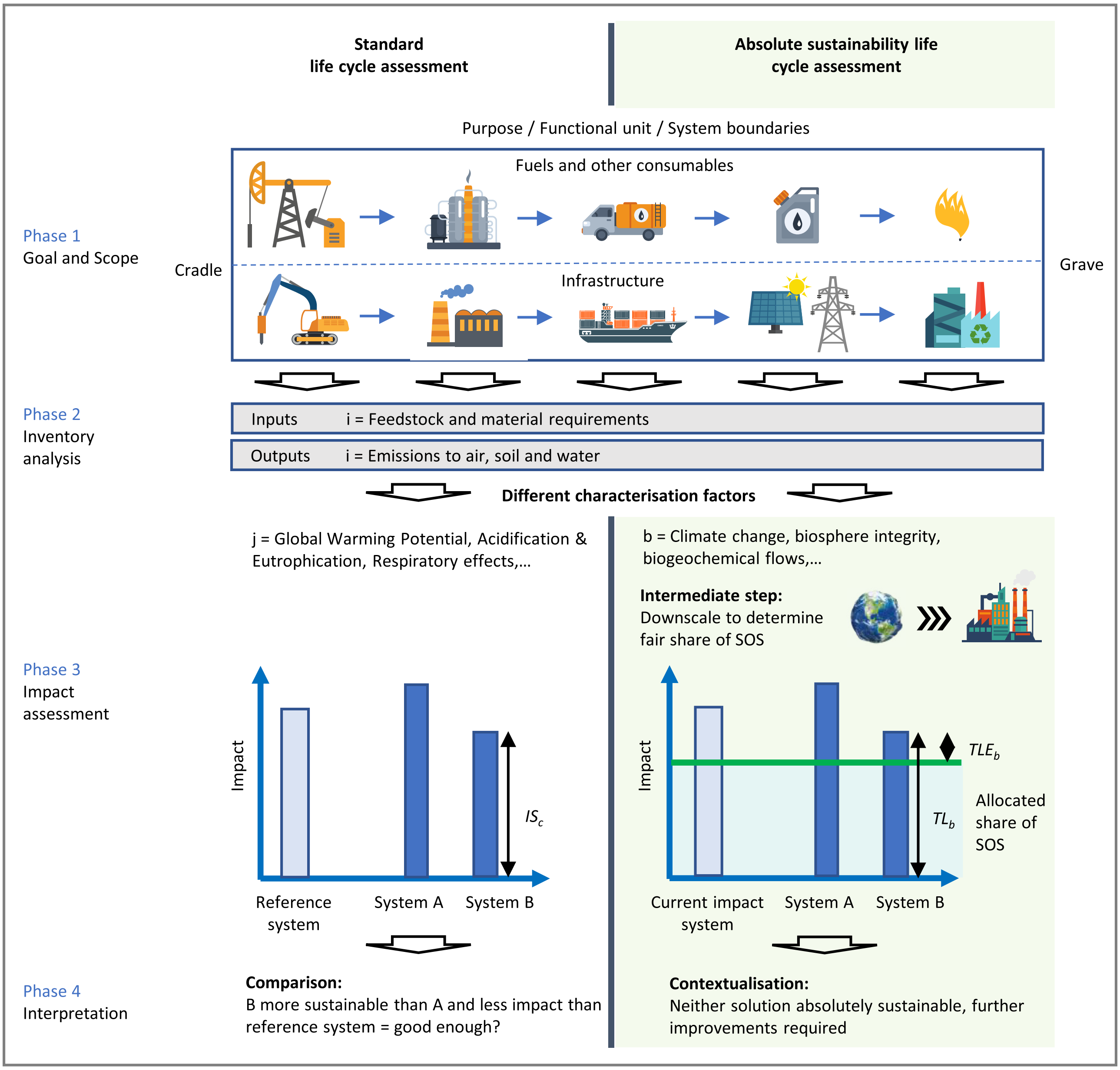

Fig. 3. The four phases of an LCA and the difference between standard LCA and an LCA that considers absolute limits for sustainability. The intermediate step, downscaling, to determine the allocated share of safe operating space (SOS) is optional and often used to operationalise absolute environmental sustainability assessments.

lution or predefined scenarios. The second alternative, which (arguably) entails a stronger interaction, follows a life cycle optimization approach (Azapagic, 1999) where life cycle impact data are incorporated into the optimization model, allowing to optimize the system for the lowest impact configuration. These data can be in the form of the life cycle inventories or impact values of some activities connected to the foreground system. These can include various types of infrastructure and all potential fuels, whose LCA data are often extracted from LCA software/databases and incorporated into the optimization model via parameters. A more sophisticated approach yet to be explored would entail combining input-output LCA data with an optimization engine (e.g. in Python through the Pyomo and Brightway packages) to optimize activities in the background and foreground systems simultaneously. Steps 2 and 3 in a standard LCA study are therefore often done concurrently in the LCO framework and linked dynamically to the optimization of the decision variables in the foreground system. Notably, impact values per functional unit of the activities linked to the foreground system are often expressed as fixed parameters added to the optimization model in the matrix of technical coefficients. Finally, the interpretation of results (step 4) is carried out in the post-optimal analysis of the Pareto solutions (Wheeler et al., 2018), which may employ multi-criteria decision-making methods.

In evaluating energy systems, it is critical to use robust data. Unfortunately, it is very challenging to gather precise data on all the echelons in the life cycle of the product under study. To circumvent this limitation, it is standard practice to rely on LCI databases containing information on a wide range of industrial activities, such as ecoinvent (Treyer and Bauer, 2016). Hence, correctly matching the components of the energy model with the appropriate activities in the LCI database is essential to produce reliable results. To this end, consistent technology classification and spatial differentiation need to be considered, so the selected database technologies are as representative as possible (Cheng et al., 2017). Even so, LCI entries are affected by uncertainties linked to data gaps and inaccuracies in the spatial, temporal and technological representation of the energy systems under assessment. Uncertainties in the LCI are commonly dealt with through a sensitivity and uncertainty analysis. Here, the major sources of uncertainty are identified and the uncertainty is sought reduced via additional data collection to improve the representativeness of the LCI. Different analytical and sampling based numerical approaches exist for this (Groen et al., 2017). Another common approach for addressing uncertainty in the LCI is the Pedigree matrix (Ciroth et al., 2016). The Pedigree matrix assumes that the LCI entries can be described by lognormal probability distributions whose parameters are obtained from qualitative information on the quality of the data available. From these distributions, a Monte Carlo sampling method can be run to generate plausible values of the uncertain parameters for which the LCA calculations are repeated to report confidence intervals on the impact values.

Multiple databases can be used to extract LCI data or define new activities, e.g. for novel technologies, based on existing entries, e.g. material, services, and inputs required. LCI data often combine other previously carried out LCAs of individual products and services (e.g. transporting 1 tonne over 1 km distance with a 15-tonne truck) that in turn rely on other LCA results (e.g. constructing 1 km of road). The background processes behind those entries are often predefined for a product in a given region, as typical local market mixes of inputs are used (e.g. electricity sourced from national grids in a specific year). When defining foreground processes, we need to specify their exchanges of mass and energy with the eco- and techno-sphere, e.g., amount of water consumed or fuel burned. The largest databases are ecoinvent and GaBi but other non-commercial alternatives relevant for energy systems exist, including the Environmental Footprint database, the U.S. Life Cycle Inventory Database, bioenergiedat, Probas, GREET, European reference Life Cycle Database (ELCD) and Needs (nexus.openlca.org).

Each activity in an LCI has a range of environmental interventions i , such as flows into waterways, emissions to air, land occupation, and mineral or fossil resources required, also called elementary flows (E_i). These elementary flows are assessed according to the degree to which they contribute to a specific impact category c, representing environmental issues of concern, e.g. freshwater eutrophication (Hauschild et al., 2018). The linkage of elementary flows with impact categories is achieved through characterization factors ($CF_{c,i}$). The characterization factors are derived using environmental characterization models, which describe the mechanisms from emission flow to impact for the relevant impact categories (e.g. from emissions over fate in the environment to the exposure and effect on ecosystems). Note that many substances have no effect on a certain impact category, hence $CF_{c,i}$ can be zero for them. The total impact (Eq. 1) is determined from life cycle inventories via characterization factors $CF_{c,i}$ that quantify the impact score (IS_c) in each category c per unit of flow i.

$$IS_c = \sum_i CF_{c,i} E_i \qquad \forall c \tag{1}$$

Each life cycle impact assessment (LCIA) methodology may consider different impact categories or units of reference and thus has different characterization factors to convert the elementary flows into the corresponding impact categories. Several LCIA methodologies are available (Wu and Su, 2020), which express the impacts using Midpoint or Endpoint categories. Midpoint categories are "links in the cause-effect chain (environmental mechanism) of an impact category [...] at which characterization factors or indicators can be derived to reflect the relative importance of emissions or extractions"(Bare et al., 2000). An example of a midpoint category is global warming potential, where characterization factors describe how much energy a greenhouse gas will absorb over time, relative to carbon dioxide, which is chosen as the reference value for the global warming potential. The indicator for the midpoint category is ideally selected at the point after which the mechanism is identical for all flows assigned to that impact category (Hauschild and Huijbregts, 2015). The Endpoint categories reflect the impact on the final element in the cause-effect chain, typically human health, ecosystem quality and resource depletion, which are referred to as the three areas of protection in LCA (Pennington et al., 2004). As stated in the introduction, it is not possible to derive from the Midpoint or Endpoint metrics as such whether a product, service or system can truly be considered sustainable (Fig. 3). To take the thresholds of pollutant concentration or resource use into account that maintain resilient socio-ecological systems, carrying capacities – or planetary boundaries – need to be considered (Bjørn et al., 2015). This approach is explained in the next section in detail.

2.4. The concept of planetary boundaries applied to life cycle assessments of energy systems

The concept of absolute sustainability provides an alternative general framework to quantify the impact of energy systems relative to the Planet's carrying capacity. Nine core planetary boundaries have been defined (Rockström et al., 2009), including climate change, ocean acidification, stratospheric ozone, global phosphorus and nitrogen cycles, atmospheric aerosol loading, freshwater use, land system change, biosphere integrity, and novel entities such as persistent chemicals and plastic waste. Only the first three are truly global and location-independent; the others possess increasingly local thresholds. The local exceedance of thresholds can erode resilience locally. Multiple local exceedances can become a global concern at the aggregate level or the aggregate of local exceedances may increase the likelihood of crossing planetary thresholds in other Earth system processes. For these Earth-system processes, zones of uncertainty have been defined in which the risk of impacts increases (yellow) and danger zones in which there is a high risk of serious impact (red). Although relying on the same scientific concepts, different terminology for the boundaries has been used, resulting in slightly different ways of measuring and quantifying risk zones (Chandrakumar and Mclaren, 2018). Recently, attempts have been made to include human health aspects, alongside the geophysical boundaries, putting a ceiling on acceptable disease burden to maintain adequate well-being and social stability (Sala et al., 2020). These approaches have in common the use of control variables (e.g. atmospheric CO_2 concentration or the amount of forest land lost), which are used to measure the extent of the boundary transgression.

The application of these concepts in combination with LCA helps to shed light on the absolute sustainability of diverse systems. The crucial step is to connect elementary flows (E_i) with the control variables of the respective planetary boundaries (b) by determining new characterization factors ($CF_{b,i}$) and thus impact scores (Eq. 2), akin to the relative LCIA methodologies described earlier.

$$IS_b = \sum_i CF_{b,i} E_i \qquad \forall b \tag{2}$$

First attempts to find characterization factors have been made related to the original planetary boundary concept (Ryberg et al., 2018b), and also based on the Environmental Footprint LCIA Methodology (Sala et al., 2020). These works follow two different approaches. The first is to quantify the impact of each emission type on the control variables of the PB, account for the temporal aspect of the SOS and then use these thresholds to determine the absolute sustainability level. For example, annual CO_2 emissions are converted to the equivalent increase in atmospheric CO_2 concentration, for which a limit has been defined in the PB framework. In this case, the planetary boundaries-specific characterization factors need to be directly linked to the inventory flows (Ryberg et al., 2018b), essentially constituting a new LCIA method. Alternatively, it is also possible to define absolute annual thresholds on existing LCIA metrics based on the carrying capacity concept, e.g. as shown in Sala et al. (2020) for the Environmental Footprint method, avoiding the computation of impacts on the PB's control variables. Planetary boundary and carrying capacity control variables are provided as environmental states (e.g. ppm CO_2) or flow rates (e.g. Tg N per year) while elementary flows are typically modelled in product LCAs as a single occurrence (e.g. 1 kg of coal burned or one power plant built). In AESA, each product or service needs to be described as an ongoing activity. This often requires the functional unit description to change from "X kg of coal burned for power generation for 10 years" to "X kg of coal burned per year for power generation". Such a change in the definition of the functional unit is needed because LCA results are otherwise integrated over time (Heijungs, 1995), where impacts that occur over a period that can span thousands of years (in the case of e.g., landfill leachate) are aggregated into a single impact score. The PBs are expressed in indicators of annual flow rates or environmental states (such as ppm CO_2 concentration in the atmosphere). To address these temporal constraints in conventional LCAs, and allow for expressing results in the metrics of the PBs, the elementary flows must be expressed as annual emissions (Guinée et al., 2022; Ryberg et al., 2018b).The implications for ESM are that some information is needed on the trajectory of developments, e.g. for a multi-year study the amount of coal burned per year for each year in the future needs to be known. Note that the impact score of longer lasting activities, such as infrastructure deployment (if not already included as part of the fuel activity), should be annualised (e.g. divided by the lifetime or using a discount factor). This prevents implicit disfavouring of infrastructure investments that reduce emissions over a longer time horizon, compared with more polluting but existing infrastructure.

Regarding the normalization of impacts (i.e. putting them into context), the planetary boundary concept brings decisive advantages compared with the relative LCIA methodologies illuminated earlier (Bjørn and Hauschild, 2015). For global systems, the safe operating space SOS_b can straightforwardly be used to determine the transgression level TL_b of each category as shown below (Eq. 3), providing a sound basis for expressing impact values relative to the Planet's carrying capacity.

$$TL_b = \frac{IS_b}{SOS_b} \quad \forall b \tag{3}$$

The SOS_b can either be defined on an annual basis (e.g. kg CO_2/year) or describe an allocated target, e.g. in the case of the remaining GHG emissions budget (e.g. Gt CO_2 to stay within 1.5°C) or maximum environmental state level (e.g. 350 ppm CO_2 as given in the planetary boundaries framework). Recent studies have been conducted that assess the portion of the SOS occupied by a particular activity or system, such as chemicals production (Galan-Martın et al., 2021) or heavy transport (Antonio Valente et al., 2021). This approach studies the impact of a specific system or sector at the planetary level, followed by a discussion about the contribution of the system or sector to operate within the PBs, potentially helping to direct impact mitigation efforts. A complement to this approach has been called "upscaling", where the impact of an activity or sector is extrapolated to all of humanity, addressing explicitly the question "how many Earths would we need if everyone behaved like this" (Cranston and Steffen, 2019). Often it is necessary to operationalize the concept to smaller scales, where it might be necessary to downscale the SOS, particularly when optimizing systems (see Fig. 4). This is helpful to explicitly assess if a system can be considered absolute environmental sustainable and incorporate the boundaries as a constraint or reference point into a model.

There are multiple options for downscaling bio- and geophysical global boundaries to countries, industries or activities, including individual rights or egalitarian (downscaling by population), historical rights or grandfathering (downscaling by current emissions), and utilitarian or outcome-based approaches (downscaling by value added to human beings). These are, however, inherently controversial as they introduce normative and justice considerations that cannot easily be reconciled (Ryberg et al., 2020). For example, dividing the "boundary allowance" by the global population neglects historical damages by more developed nations, geographical (dis)advantages, and unequal capital distribution (required to invest in cleaner technologies) (Häyhä et al., 2016). Nevertheless, downscaling allows assessing the absolute sustainability level of systems on a smaller and practical scale relevant for decision-making (Sandin et al., 2015), which is also useful in energy systems modeling. Previous studies have used downscaled or allocated safe operating space threholds $aSOS_b$, most typically by a combination of ratios between regional (POP^{region}) and global (POP^{world}) population (Eq. 4)

$$aSOS_b^{region} = \frac{POP^{region}}{POP^{world}} SOS_b \quad \forall b \tag{4}$$

and contributional share of an industry or activity in economic terms, using gross value added (GVA, Eq. 5) or revenue (Eq. 6) and gross domestic product (GDP) (Ryberg et al., 2020). GVA excludes intermediate consumption (of inputs), hence the choice of the economic indicator depends on the scope of the environmental assessment, e.g. whether supply chain emissions (Scope 3) are included (Hertwich and Wood, 2018), where Scope 1 means that only direct emissions during production are accounted and Scope 2 additionally includes the impacts of the electricity consumed.

$$aSOS_b^{activity} = \frac{GVA^{activity}}{GDP^{world}} SOS_b \quad \forall b \tag{5}$$

$$aSOS_b^{activity} = \frac{revenue^{activity}}{GDP^{world}} SOS_b \quad \forall b \tag{6}$$

Transgression levels can be derived for a range of Earth system processes. The question then is how to define a comprehensive objective function to drive the optimization of energy systems capitalizing on such multiple variables. For global or downscaled smaller systems, employing the transgression level excess TLE_b (Eq. 7) can help design absolute sustainable systems.

$$TLE_b = \max\{1, TL_b\} - 1 \quad \forall b \tag{7}$$

A maximum TLE_b of 0, i.e., operating within the SOS, can be introduced as a hard constraint in an optimization model, allowing to optimise for a single objective (e.g. economic) only while not exceeding the allowable ecological budget. This type of problem resembles a standard flexibility analysis or robust optimization problem where a solution is sought that can operate within a feasibility range (Zhang et al., 2016). Alternatively, TLE_b can be appended to the objective function, so the model minimizes the transgression level, potentially together with other metrics, and thus only penalizes impacts above the carrying capacity (Vázquez and Guillén-Gosálbez, 2021).

The complexity of multi-objective problems drastically increases with the number of objectives. Notably, simultaneously optimizing nine or more variables, i.e., the total number of PBs, would be computationally intensive, so alternative approaches are required to enable a comprehensive and numerically efficient optimization of sustainability criteria in an absolute context. A straightforward approach is to optimize for the maximum transgression using the maximum value of TL_b (TL^{max}, Eq. 8) as the ob-

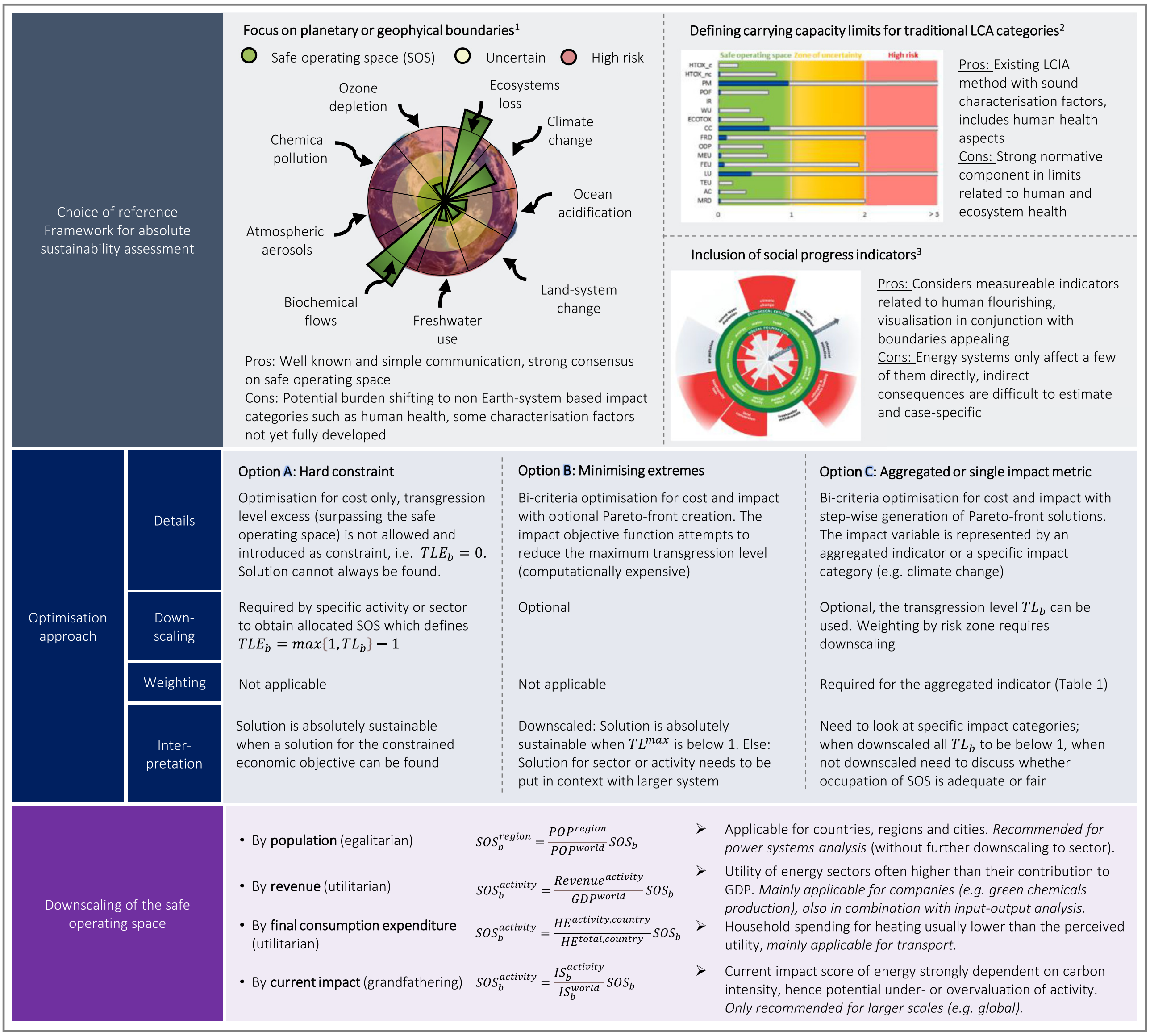

Fig. 4. Overview of methodological choices when conducting an absolute sustainability LCA for ESM. Examples for the reference frameworks can be found in 1: Rockström et al. (2009a), 2: Sala et al. (2020) and 3: Raworth (2017) .

jective (Eq. 9). This reflects a precautionary approach focusing on the most critical transgression level.

$$TL^{\max} \geq TL_b \quad \forall b \tag{8}$$

$$\min\{TL^{max}\} \tag{9}$$

The alternative is to aggregate the TL_b or TLE_b values of all boundary categories into a single metric, e.g. an absolute sustainability indicator, *ASI*. This requires a weighting vector (W_b)Vargas-Gonzalez et al., 2019), so the objective function would then minimize an aggregated transgression metric *ASI* (Eqs. 10 and (11).

$$ASI^{TL} = \sum\nolimits_b TL_b W_b \tag{10}$$

$$ASI^{TLE} = \sum\nolimits_b TLE_b W_b \tag{11}$$

Note that net-negative contributions to a boundary (TL<0), e.g., sequestering carbon, would not compensate for burdens in other categories when using TLE_b, unlike when using TL_b. Different approaches to weighting in the context of planetary boundaries are listed in Table 1 and their suitability depends on the study design and objectives. Weighting and single indicators are inherently problematic as a) the choice of a weighting vector can never capture the exact relevance and urgency (i.e. hierarchy) of the planetary boundaries at a given point in history and geographical location, and b) low impacts in some categories can mathematically compensate for high impacts in other categories, which is incoherent with processes in the natural world. Nevertheless, in some situations, e.g. when downscaling is not practical or when a truly sustainable solution cannot be found, weighting needs to be resorted to. Fig. 5 depicts a potential sequence that could be followed to formulate an optimization model accounting for absolute sustainability criteria. Further discussion on allocation (downscaling) principles and category aggregation can be found in Bjørn et al., 2019.

As stated previously, the LCA-PB approach can be applied retrospectively as a post-processing step to results of existing ESM, IAM or any other previously conducted studies (Child et al., 2018).

Table 1
Different approaches to weighting absolute sustainability impact categories when using an aggregated impact metric in mathematical optimization. The domain of each equation is the set b, planetary boundary categories.

Method	Equation	Details
Average or equal relevance	$W_b = \frac{1}{\lvert PB \rvert}$	The weighting factor is the same for each category and adds up to 1 for all categories, determined by the number of planetary boundary categories considered ($\lvert PB \rvert$).
Based on current transgression levels	$W_b = \frac{\frac{IS_b^{current}}{SOS_b}}{\sum_b \frac{IS_b^{current}}{SOS_b}}$	The current impact of the anthropogenic activity of a system is chosen to determine the weighting factor. This may be used when some categories are already in a high-risk zone where impact reduction is more urgent. Naturally, this requires knowledge of current impacts in all categories (see Bjørn and Hauschild (2015), O'Neill et al. (2018) or Sala et al. (2020) for annualized per capita values).
Based on actively minimizing extremes	$W_b = \frac{TL_b}{MEAN(TL_b)} * \frac{1}{\lvert PB \rvert}$	This approach compares all the values in each impact category and lends a higher weight to categories for which the transgression level is above the average, thus actively attempting to equalize the environmental pressures the system under study is causing. This introduces non-linearity to the model and is computationally costly. Note that TL_b can't be replaced here by TLE_b as fully sustainable systems would cause a division by zero.
Based on the average current transgression level	$W_b = \frac{\frac{IS_b}{SOS_b} * \frac{1}{\lvert PB \rvert}}{MEAN(\frac{IS_b^{current}}{SOS_b})}$	This is similar to minimizing extremes but utilizes a comparison with the average current transgression level to weigh each category, thus passively attempting to equalize environmental pressures. This also introduces non-linearity but does not continuously compare intermediate results and is less computationally costly.
Based on risk zones	$TL_b < 1;\ W_b = \frac{1}{\lvert PB \rvert} * 1$ $TL_b > 1;\ W_b = \frac{1}{\lvert PB \rvert} * X$	Multiple weighing factors according to the risk zone of the planetary boundary Wheeler et al. (2021). Transgressed categories receive a higher weight (factor X, >1). Introduces additional complexity to the model.

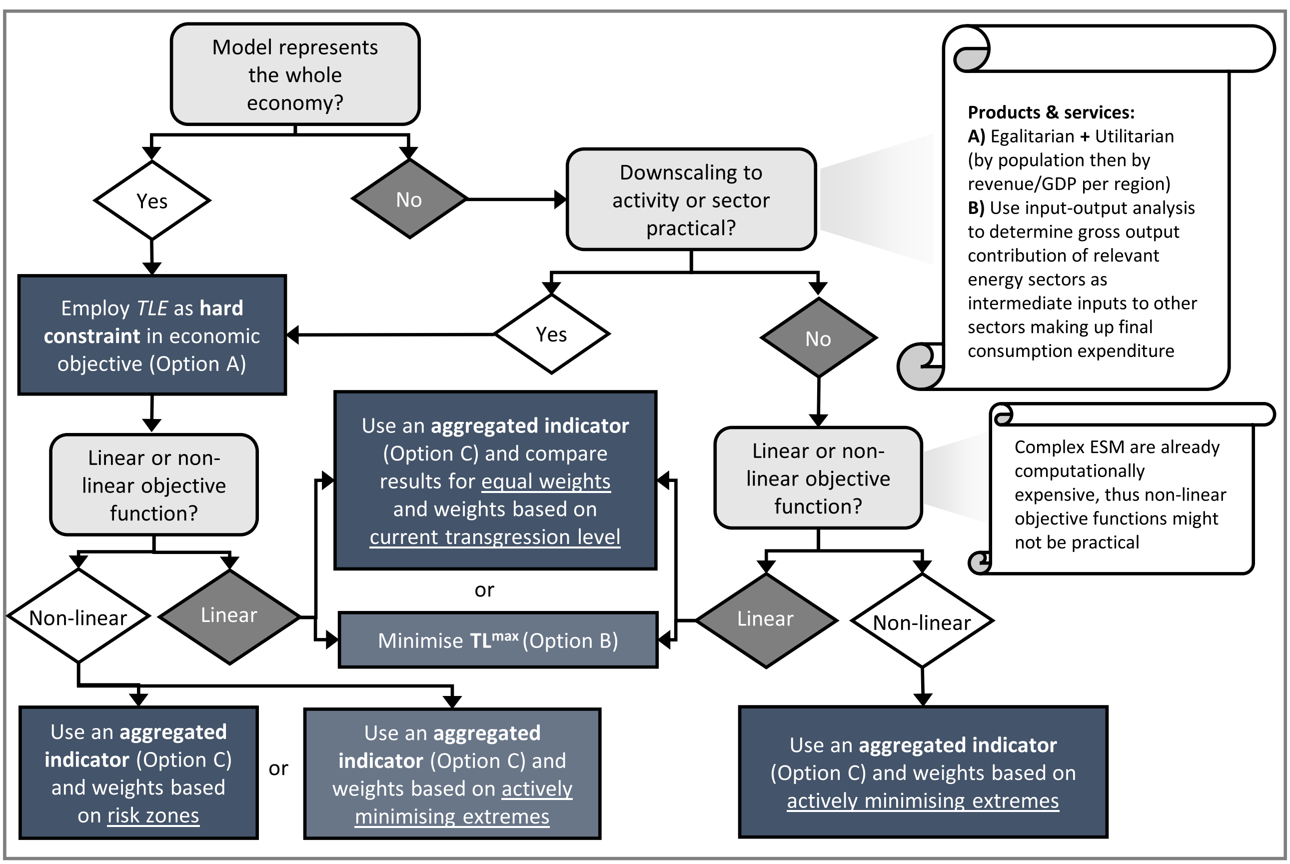

Fig. 5. Recommended heuristics for incorporating AESA into ESM models. Downscaling by population to the target geography of inquiry is always recommended as a first step. Options are further detailed in Fig. 4 and weighting methods are explained in Table 1. In the long term, there is a need to develop widely agreed, case-sensitive and practical downscaling frameworks for ESM.

Recently, studies have started to incorporate the above-mentioned concepts, combining optimization with LCA-PB in the wider energy systems realm. For the US, it was shown that a cost-optimized power system that achieves the 2°C Paris target transgresses several planetary boundaries and thus cannot be considered absolutely sustainable, while a transgression-minimized power system would cost almost twice as much (Algunaibet et al., 2019b). Least-transgression scenarios were developed for green methanol production in China, where transgression could be greatly reduced compared with the business as usual (BAU) case at similar economics (Yinan Li et al., 2020). In the context of supply chain design for transport fuel, it was found that different technologies and logistical arrangements are chosen when considering planetary boundaries for a hydrogen economy in the UK (Ehrenstein et al., 2020) or for a bioethanol supply in Argentina (Wheeler et al., 2021). In the latter study, different downscaling mechanisms also affected the system design due to more or less stringent boundaries highlighting the sensitivity of the results to the downscaling principle. On a smaller scale, Vázquez and Guillén-Gosálbez (2021) optimized the electricity supply for a methanol production plant and identified strong cost and transgression trade-offs between different hydrogen production technologies.

Most of these studies downscaled by GVA to GDP ratios, employed equal weights for each boundary and optimized for the transgression level excess, TLE_b. Sometimes, downscaling by the share of the current impact of the activity was chosen ("grandfathering") or the impact has been put in context with the global boundaries, omitting the downscaling step (Antonio Valente et al., 2021). Most of the studies mentioned above optimized the economic and environmental function separately, constructing a Pareto curve for different solutions applying the ε-constraint method (Guillen-Gosalbez et al., 2007). Here, values of the absolute sustainability indicator provide the lower (following optimization of the environmental function) and upper bound (following optimization of the economic function) and the system is consecutively optimized for minimum cost at different impact constraints between those bounds (Guillén-Gosálbez et al., 2019).

Although the LCA-PB method enriches energy systems sustainability assessments, design tasks and international negotiations, many challenges and uncertainties remain, which require further methodological and scientific advancements (Table 2).

3. Challenges in environmental assessments of energy systems

3.1. Selection of an adequate boundary framework

The PB framework proposed by Rockström et al. (2009) is limited to bio- and geophysical boundaries, it thus pertains only to critical aspects of maintaining the Earth system processes and disregards crucial factors for human flourishing, such as the impacts on human health or unsustainable resource extraction. Furthermore, no social indicators are considered that represent the needs of people, such as access to electricity (O'Neill et al., 2018). Those aspects, however, are relevant for energy systems and might present critical trade-offs, e.g. a coal power plant providing electricity but causing health issues due to particulate matter. On the other hand, if non-geophysical factors are omitted, optimizing to prevent ecological overshoot might compromise social outcomes (Fanning et al., 2021). Currently, no framework exists that can be considered holistic, though attempts have been made to link the Sustainable Development Goals (SDG) with the PB framework (Chandrakumar and Mclaren, 2018) or to simultaneously achieve the SDGs while staying with PBs (Randers et al., 2019). The carrying capacity method developed by Sala et al. (2020) includes, besides bio- and geophysical aspects, human health and resource use impacts. Nevertheless, issues arise due to the more subjective nature of some categories, e.g. what can be considered an "acceptable disease burden", compared with a more scientific understanding of ecological limits. An approach complementing the PB framework is the Doughnut (see Fig. 4), which includes besides the SOS a "just operating space", where several basic human needs are being met (Raworth, 2017). Despite its advantages, its applicability for ESM is limited as only a few of the need categories are directly impacted by energy systems. Recommendations for practitioners and future research are listed in Table 2 for this and the following subsections.

3.2. Definition of relevant control variables and risk zones for less defined boundaries

The community around the PB framework has yet to agree on control variables for the boundary categories aerosol loading (Steffen et al., 2015). The novel entities category (e.g. persistent chemicals, engineered nanoparticles and marine plastic) has recently been quantified using a set of characterization factors (Persson et al., 2022), but it still lacks an agreed definition of which substances are included (Li et al., 2021) and knowledge gaps exist about their impacts(Villarrubia-Gómez et al., 2018). Attempts have been made to refine the control variables for practical use, for example, by implementing proxy characterization factors for biosphere integrity affected by land use and global warming (Hanafiah et al., 2012). It still remains a challenge to adequately account for the loss of functional and genetic biodiversity. Further, the quantification of the safe operating space, i.e. when the safe operating space has been breached, is not yet fully developed or agreed upon for all categories, such as biosphere integrity (Montoya et al., 2018) or freshwater withdrawal (Bunsen et al., 2021). The definition of risk zones follows the precautionary principle as different countries or cultures might interpret risk in various ways. Wealthy nations with sufficient capital to invest in adaption technologies likely interpret risk differently than poorer nations with geographically unfavorable vulnerabilities. The characterization factor developed for the boundary for climate change currently depends on the ambition, a 1.5°C target results today in 0.985 tonne CO_2 and a 2°C target in 1.61 tonne CO_2 per person per year (Ryberg et al., 2018b). There are also interactions between boundaries, which are not yet fully understood and could increase the risks (Lade et al., n.d.). There are thus significant uncertainties when modeling and interpreting the impacts in those categories. Nevertheless, the classification of climate change and biosphere integrity as core boundaries introduces a hierarchy at least from an Earth system processes perspective. For the other boundaries, the criticality depends on more local conditions.

3.3. The need for sub-global scales and thresholds

Only climate change, ocean acidification and stratospheric ozone are truly planetary-scale processes (Rockström et al., 2009). The Earth system processes in the PB framework are aggregated from small spatial scales. For those sub-global boundaries, an exceedance of the local carrying capacity cannot adequately be captured by the global control variable (Biermann and Kim, 2020). For example, excessive nutrient flows into a river basin might lead to a collapse of the local ecosystem. Further, the current SOS for freshwater consumption has been criticised to inadequately portrait the already critical situations in many parts of the world (Pfister and Ridoutt, 2015).

Energy system studies are often place-specific to account for the renewable energy resources and demand profiles, hence local thresholds are particularly relevant. First attempts have been made to localize some of the characterization factors (Verones et al., 2020; Ryberg et al., 2021). This seems particularly promising for biosphere integrity, as the species richness in specific areas is known and can be used to create high-resolution characterization factors (de Baan et al., 2013). Another approach is to use available category-specific indicators to define the criticality of the boundary category in a specific region, e.g. the aridity index (Trabucco et al., 2019) for the freshwater use boundary. A slightly different angle to considering local limits within ecosystems is the valuation or accounting of ecosystem services (ES), such as clean air or water provisioning, which can be included in economic assessments (Garcia and You, 2018). ES can be linked to life cycle impact as-

Table 2
Overview of current challenges when applying absolute sustainability concepts to ESM and recommendations for practitioners and future research.

Challenge	Recommendation for practitioners	Recommendation for future research
Selection of an adequate boundary framework	• Tailor framework to the goal (e.g. does the energy system affect multiple social categories?) • Complement PB with standard LCIA methodologies including human health categories if possible to reveal potential trade-offs or co-benefits beyond the Earth system processes	• Evaluation of existing frameworks for ESM; identifying pressing human welfare aspects often overlooked and experiencing burden shifting when optimizing only for geophysical boundaries
Definition of relevant control variables and risk zones for less defined boundaries	• LCA-PB complementary to standard LCA reporting (mid/endpoint) • Future ESM to account at least for biosphere impacts on top of global warming when considering bioenergy	• Interdisciplinary definition of control variables and quantification of SOS for missing categories • Refinement of the biosphere integrity categories as affected by energy systems • Updating of characterization factor for climate change to actual global emissions trajectory over the last few years
The need for sub-global scales and thresholds	• Simultaneous consideration of global boundaries and known local thresholds or acceptable limits	• Development of open-access GIS-based characterization factors or control variable values
Complexities of downscaling the safe operating space for energy systems	• If possible, use input-out tables to obtain impact contribution of energy within all sectors, if not downscale by population and then value added for products and services • Potentially employ different downscaling methods and compare the results • Clearly state and justify which justice theory or downscaling approach was chosen	• Development of widely agreed, case-sensitive downscaling framework
Solving multi-objective optimization problems	• Ideally, use downscaling combined with hard constraints on boundaries (only economic optimization), otherwise use an equal weighting approach or weighting by the most critical boundaries for the case study and generate a Pareto curve with dual- or triple-objective optimization • Clearly state rationale and limitations of the chosen approach	Further investigate hierarchy, criticality, and interactions of PB categories to provide some guidelines on justifiable weighting approaches depending on the case study
Modeling and optimization under data uncertainty	• Use sampling methods or scenarios for the most critical and variable input data • Clearly state that outcomes are subject to variability, which could not be adequately assessed by the model	• Develop stochastic optimization methods and tools that can incorporate parameter ranges • Develop standards for accounting for parametric uncertainty
Shortcomings of integrated assessment models	• Increase transparency about techno-political assumptions used in own model or employ different scenarios • State assumptions of underlying data used to generate future-oriented LCI data • Data and model open-source	
Effective reporting on multiple impact categories, scenarios and objectives	• Consider the target audience and stakeholder communication needs • Learn and employ novel and creative visualization techniques while maintaining scientific accuracy	

sessments (LCIA), where the changes on ecosystems due to human impacts change the quality and/or quantity of supplied ES (Rugani et al., 2019). The incorporation of ES into system optimization can significantly influence supply chain design and operations decision-making (Ghosh and Bakshi, 2019). Although ES accounting requires different methods and information compared with the PB framework, it can help to establish local thresholds for specific localities (Vargas et al., 2017). Besides thresholds founded in natural science, communities or countries might define socially acceptable limits where risk is accepted to some degree, as has been done with air pollution for example (Huang et al., 2017). A major challenge to defining such acceptable limits is that different stakeholders have different needs; indigenous communities and energy companies might have competing interests, calling for mediation and a joint approach (Moomen and Dewan, 2017). This can complement the efforts of scientists and calls for inclusive approaches, e.g. by including state actors, provided they are not biased.

3.4. Complexities of downscaling the safe operating space for energy systems

ESM usually consider a defined spatial extent, such as a region, country or city. As such, it can be favorable for results interpretation and constrained optimization to downscale the global SOS to the respective scale. The different approaches to allocating a share of the boundary and their application have been described elsewhere (Ryberg et al., 2020). The issue that geographically-bound ESM face is that there is no ideal approach to allocation for several reasons. First, energy is essential in virtually all sectors of the economy, in particular heavy industry, but its contribution to economic output cannot easily be quantified. Considering the power sector, this means that applying economic downscaling by contribution to GDP or household spending results in unrealistically small allocations. Second, the impact of energy provision depends strongly on the current system design. The grandfathering approach, which allocates the share of SOS according to the current share of emissions, would result in a larger allowance for "dirty" energy systems. Third, the utility of energy to a populace is difficult to quantify, as subsistence consumption is taken for granted, and thus the perceived value can be lower compared with luxury consumption (Bucchianico et al., 2021), necessitating deeper studies into marginal utility. Thus, downscaling to sectors or activities using utilitarian or historic approaches is so far mainly recommended for final products, not intermediate products such as energy used within the industry. One reason is to prevent double counting, as the energy input to other sectors is often accounted for in those sectors. For geographically-bound models the only moderately justifiable approach is the egalitarian one, allocating SOS by population share. One way to tackle this problem is to build models that portrait the whole world (Randers et al., 2019), naturally compromising on accuracy and validity.

A more promising approach to include intermediate products is to assign an economic share to intermediate products, such as energy, based on their contribution to the final products and, thus, the indirect value to final users (e.g. households and governments). Environmentally extended multiregional input-output (EE-MRIO) models (Stadler et al., 2018) could be used to create an overview of the global economy and the interlinkage between industrial final and intermediate products and sectors. A simplified and similar approach is a combination of regionalization and economic relevance, i.e. first downscaling the global boundary to the national or regional population, then dividing the revenue of the sector or company (achieved within the geographical area) by the GDP of the geographical area. This ensures fairness between poorer and richer countries and uses readily available data for economic allocation. It can also be applied for globally operating companies, as their revenue is often reported by region, where the company's allocated SOS is the sum of allocated SOS for each regional activity of that company. Still, the indicators on which to assign a share to intermediate products (e.g. revenue, number of employees, environmental impacts, marginal wellbeing for consumers) is still highly debatable, and the selection of one set of indicators will inevitably favor some industries at the expense of others. Thus a general issue with regards to downscaling and assignment of the safe operating space is the selection of appropriate and generally accepted indicators. We provide recommendations related to downscaling in Fig. 5, but acknowledge the issue and potential controversy related to downscaling and that further research is still needed on this subject. Thus, transparency and documentation of the downscaling approach are essential to ensure openness about the choice of downscaling methodology and the value-based choices pertaining to this.

3.5. The need for harmonized and prospective life cycle inventories

The use of existing LCI databases is indispensable when conducting energy systems modeling. However, current databases rely on LCA studies that have been conducted in the past and often with limited transparency about the assumptions. Frequent updates of the databases reveal how much the impacts of activities change over time (Vandepaer et al., 2019). Particularly the provision of low-carbon technologies, e.g. solar photovoltaic, is currently carbon-intensive – due to the electricity mix used in the production – and carbon intensities for energy generation are thus projected to change significantly (Pehl et al., 2017). There are thus issues around the timeliness and trustworthiness of the data. To tackle the timeliness, efforts have been made to keep databases up-to-date and create databases that consider technologies deployed in the future (Sacchi et al., 2021) and make these accessible to everyone (Steubing et al., 2020). However, this introduces a range of new uncertainties discussed in Section 4.3.

4. Computational and practical challenges in absolute sustainability assessments

4.1. Solving multi-objective optimization problems

Optimizing ESM for more than just economics inevitably introduces challenges and options for solving a model and generating results (Fig. 4). In the context of the PB framework, the practitioner may want to minimize the impact in all the PBs simultaneously. The most suitable approach to deal with multiple objectives in optimization problems is by applying multi-objective optimisation (MOO) methods (Pieragostini et al., 2012). The solution of MOO is provided by a set of optimal solutions, called Pareto optimal, which represent the trade-off among the objectives considered showing conflicting behaviors (i.e. improving in one leads to worsening in the others). Although insightful, selecting the most preferred alternative among all optimal solutions is challenging and, more importantly, minimizing the pressure in one PB does not necessarily mean that the optimal system operates below the threshold (i.e. being absolute sustainable in one category but disregarding all others does not generate desired solutions). Moreover, MOO problems with more than two or three objectives (bi-criteria or three-objectives problems) also pose challenges regarding the visualization of the results and, therefore, the interpretation. Hence, in LCA studies, it is common to aggregate environmental categories in a single indicator (Guillen-Gosalbez et al., 2007), resulting in a dual-objective optimization for which a two-dimensional Pareto frontier of optimal solutions (see Fig. 2) can optionally be generated (Yue et al., 2016). This approach could also be extended to the PB framework by using aggregated transgression levels at the expense of losing information regarding each particular PB. Three-dimensional Pareto fronts can also be used when incorporating social objectives into the PB framework (Rockström et al., 2021) However, this introduces the issue that low impacts in some categories can offset the exceedance of the boundaries in others. Employing transgression level-dependent weight as described in section 2.4 could mitigate this issue .

Despite the practicality of approaches relying on aggregated indicators, they introduce controversies related to weighting between the categories, i.e. making a value judgment about their relative importance (Huppes 2011). Hence, none of the options shown in Table 1 is yet approved or recommended by a significant body of researchers or practitioners. An alternative approach for bi-criteria optimization is to reformulate the bi-criteria objective as economic, process or environmental efficiency (e.g. using profit instead of cost, divided by the impact), thus switching from a minimization to a maximization goal (Pieragostini et al., 2012). This leads to a single objective function but also to a non-linear optimization problem, which could be solved with tailored decomposition methods for fractional programming.

With an increased understanding of interlinkages between boundaries, a damage model could hypothetically be developed, condensing all Earth system process boundaries into a single indicator (e.g. stabilisation of Holocene). Although simplifying the optimisation problem, the complexity of the Earth system processes can likely not be done justice in this way, thus substantially introducing uncertainty.

Treating absolute sustainability categories as hard constraints in the formulation of the optimization model reduces it to a single-objective (usually economic) optimization problem, overcoming the limitations mentioned above, but introduces the controversies around downscaling illustrated in Fig. 4 and discussed in 3.4. These controversies around weighting and downscaling can not yet be fully reconciled for absolute sustainability assessments in ESM, thus every study needs to justify their case-specific choice of approach and clearly state the limitations.

4.2. Modeling and optimization under data uncertainty

The range of different production methods, supply chains and local conditions existing around the globe (i.e. market and technical uncertainties) leads to variability in data related to costs and impacts of infrastructure, equipment, consumables and transportation. Every entry in a database for cost and impact of activities or products either describes a very specific setup or represents an average value of multiple different setups. Thus, a more robust perspective on input data (or parameters) for a model is that of a probability density function (PDF) (Muller et al., 2018). It is possible to generate probabilistic results in most LCA software, e.g. by running a large number of possible options, or samples, to create an output PDF, using for example Monte Carlo sampling. The probabilistic approach can also be applied in optimization models using stochastic programming or robust optimization, as discussed elsewhere (Guillén-Gosálbez et al., 2019). However, this approach is challenging to implement in large optimization models due to the increase in complexity brought about by the explicit consideration of the uncertain parameters space in the optimization step. This is particularly true when various uncertainty sources need to be modeled simultaneously, including technical, market-related, and environmental uncertainties. Further, data variability is not always portrayed correctly in databases and not all software use adequate sampling methods, e.g. leading to data points with infeasible values in LCA (Lesage et al., 2018). There is a lack of harmonization and standards of how to account for data uncertainty in ESM, while existing standards for LCA are rarely adequately applied. Besides these market and technical uncertainties, there are also uncertainties related to the characterization factors, i.e. how specific outputs from the technosphere influence the planetary boundary control variables (Ryberg et al., 2016). These aspects make it currently challenging to generate and report results that adequately portray the inherent variability of the outcome.

4.3. Shortcomings of integrated assessment models used in energy systems analysis

Multi-sectorial and multi-period IAM that consider energy systems usually produce cost-optimal capacity deployment strategies to reach certain emission reduction targets (Hall and Buckley, 2016). To do this, they rely on a range of assumptions related to population dynamics, GDP growth, final energy demand and other socio-economic factors. The IAM and ESM in general also differ in the assumptions and simplifications related to technological capacity limits, deployment rates and other techno-political factors. There are a few shortcomings when using AESE in combination with IAM. First, the different assumptions can be time-consuming to identify, and paired with the complexity and size of those models, making the models difficult to access and understand for researchers outside the group that developed them (Pfenninger, 2017). Second, access to data and software is not always given but would help to validate the assumptions behind policy-influencing expert advice (Pfenninger et al., 2017). Third, the socio-economic factors, in contrast to technological assumptions, have been harmonized via the introduction of shared socioeconomic pathways (SSP) (Riahi et al., 2017), but interactions between environmental impacts and civilization, e.g. climate-induced migration, are typically underrepresented as they are non-linear and unknown (Boas et al., 2019). Lastly, IAM also constitute the data source for prospective LCA databases, such as premise (Sacchi et al., 2021). The range of potential futures and their assumptions thus influence the background data and, consequently, the results of prospective LCA studies (Mendoza Beltran et al., 2020). Energy system modelers, when using such future-oriented databases, need to be aware of the assumptions behind the data they are using and need to select the appropriate scenario for their study.

4.4. Effective reporting on multiple impact categories, scenarios and objectives

Energy systems are typically modeled to show the influence of a breadth of factors, including different constraints (e.g. climate mitigation targets), scenarios (e.g. exclusion or inclusion of certain technologies or practices), and assumptions (e.g. capacity constraints or demand projections). This alone presents challenges related to effective reporting, addressing accessibility, transparency and completeness of results (e.g. showing the total costs, energy flow and system configuration for multiple scenarios, assumptions and objectives) (Alemasoom et al., 2016). Incorporating sustainability assessments into ESM adds another dimension, not just creating new potential solutions for each scenario and set of assumptions (due to multiple objectives in the optimization) but also new requirements related to sensitivity, variability and uncertainty of results (Sala and Andreasson, 2018). There is a lack of standards or harmonization for results interpretation and visualization for LCA so far (Hollberg et al., 2021), much less for LCA-PB. On the other hand, the radar or sunburst graph depicting the PB (Fig. 4) has been widely printed and shared, potentially providing an advantage for environmental impact results presentation compared with conventional LCA (Sterner et al., 2019). Practitioners need to be aware of their target audience and tailor the visualization approach to the diverse communication needs of different stakeholders (Sala and Andreasson, 2018).

5. Conclusion

The transition to a greener energy system is of paramount importance to preserve the biosphere and the well-being of future generations. In combination with ESM, the concept of absolute sustainability can help to design not just economically favored but also genuinely environmentally sustainable solutions. AESA helps to reveal burden-shifting, preventing myopic or single-issue problem fixing in policy-making. In contrast to relative sustainability or conventional LCA, these new tools enable optimization approaches in ESM to consider a breadth of impact categories while respecting bio- and geophysical limits. They also facilitate the interpretation and communication of impact categories and modeling outcomes. Moreover, absolute normalization and downscaling, albeit imperfect, offer practical approaches to policy- and decision-relevant modeling efforts. We have identified a range of areas that require care when applying these methods and identified topics requiring further research and harmonization from practitioners and decision-makers. In particular, the inclusion of human welfare criteria, also expressed by the SDGs, further refinement of control variables, risk zones and local thresholds, and noteworthy limitations of the method that need to be communicated. Despite required refinements and harmonization, the concept can already be used in ESM and it is our hope that this work encourages further application and development to help design a sustainable energy sector and beyond.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

CRediT authorship contribution statement

Till Weidner: Conceptualization, Methodology, Visualization, Writing – original draft. **Ángel Galán-Martín:** Writing – original draft, Writing – review & editing. **Morten Walbech Ryberg:** Writing – original draft, Writing – review & editing. **Gonzalo Guillén-Gosálbez:** Conceptualization, Supervision, Writing – review & editing.

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Appendix. List of Notation

ASI Asbolute sustainability indicator

$CF_{c,i}$ Characterization factor for category c (or boundary b) and elementary flow i

E_i Quantity of elementary flow i

GVA Gross value added

GDP Gross domestic product

HE Household expenditure

IS_c Impact score for category c (or boundary b)

PB Planetary boundary

POP Population

TL_b Transgression level for boundary b

TLE_b Transgression level excess for boundary b

TL_{max} Maximum transgression level

SOS_b Safe operating space for boundary b

W_b Weight for boundary b

References

Alemasoom, H., Samavati, F., Brosz, J., Layzell, D., 2016. EnergyViz: an interactive system for visualization of energy systems. Vis. Comput. 32, 403–413. doi:10.1007/s00371-015-1186-8.

Algunaibet, I.M., Guillén-Gosálbez, G., 2019. Life cycle burden-shifting in energy systems designed to minimize greenhouse gas emissions: Novel analytical method and application to the United States. J. Clean. Prod. 229, 886–901. doi:10.1016/J.JCLEPRO.2019.04.276.

Algunaibet, I.M., Pozo, C., Galán-Martín, Á., Guillén-Gosálbez, G., 2019a. Quantifying the cost of leaving the Paris Agreement via the integration of life cycle assessment, energy systems modeling and monetization. Appl. Energy 242, 588–601. doi:10.1016/J.APENERGY.2019.03.081.

Algunaibet, I.M., Pozo, C., Galán-Martín, Á., Huijbregts, M.A.J., Mac Dowell, N., Guillén-Gosálbez, G., 2019b. Powering sustainable development within planetary boundaries. Energy Environ. Sci. 12, 1890–1900. doi:10.1039/c8ee03423k.

Anand, R., Aggarwal, D., Kumar, V., 2017. A comparative analysis of optimization solvers 20, 623–635. doi:10.1080/09720510.2017.1395182.

Andiappan, V., 2017. State-Of-The-Art Review of Mathematical Optimisation Approaches for Synthesis of Energy Systems. Process Integr. Optim. Sustain. 13 (1), 165–188. doi:10.1007/S41660-017-0013-2.

Azapagic, A., 1999. Life cycle assessment and its application to process selection, design and optimisation. Chem. Eng. J. 73, 1–21. doi:10.1016/S1385-8947(99)00042-X.

Babrowski, Sonja, Heffels, T., Jochem, P., Fichtner, W., Babrowski, S, Heffels, · T, Jochem, · P, Fichtner, · W, 2014. Reducing computing time of energy system models by a myopic approach A case study based on the PERSEUS-NET model List of symbols Indices. Energy Syst 5, 65–83. doi:10.1007/s12667-013-0085-1.

Bakshi, B.R., Gutowski, T.G., Sekulic, D.P., 2018. Claiming Sustainability: Requirements and Challenges. doi:10.1021/acssuschemeng.7b03953.

Bale, C.S.E., Varga, L., Foxon, T.J., 2015. Energy and complexity: New ways forward. Appl. Energy 138, 150–159. doi:10.1016/J.APENERGY.2014.10.057.

Bare, J.C., Hofstetter, P., Pennington, D.W., de Haes, H.A.U., 2000. Midpoints versus endpoints: The sacrifices and benefits. Int. J. Life Cycle Assess. 56 (5), 319–326. doi:10.1007/BF02978665.

Baumgärtner, N., Deutz, S., Reinert, C., Nolzen, N., Kuepper, L.E., Hennen, M., Hollermann, D.E., Bardow, A., 2021. Life-Cycle Assessment of Sector-Coupled National Energy Systems: Environmental Impacts of Electricity, Heat, and Transportation in Germany Till 2050. Front. Energy Res. 0, 27. doi:10.3389/FENRG.2021.621502.

Biermann, F., Kim, R.E., 2020. The boundaries of the planetary boundary framework: A critical appraisal of approaches to define a "safe operating space" for humanity. Annu. Rev. Environ. Resour. 45, 497–521. doi:10.1146/annurev-environ-012320-080337.

Bisschop, J.J., Entriken, R., 1993. AIMMS: The Modeling System. Paragon Decision Technology B.V. https://doi.org/10.2/JQUERY.MIN.JS.

Bjørn, A., Chandrakumar, C., Boulay, A.-M., Doka, G., Fang, K., Gondran, N., Hauschild, M.Z., Kerkhof, A., King, H., Margni, M., McLaren, S., Mueller, C., Owsianiak, M., Peters, G., Roos, S., Sala, S., Sandin, G., Sim, S., Vargas-Gonzalez, M., Ryberg, M., 2020. Review of life-cycle based methods for absolute environmental sustainability assessment and their applications. Environ. Res. Lett. 15. doi:10.1088/1748-9326/ab89d7.

Bjørn, A., Diamond, M., Owsianiak, M., Verzat, B., Hauschild, M.Z., 2015. Strengthening the Link between Life Cycle Assessment and Indicators for Absolute Sustainability To Support Development within Planetary Boundaries. Environ. Sci. Technol. 49, 6370–6371. doi:10.1021/acs.est.5b02106.

Bjørn, A., Hauschild, M.Z., 2015. Introducing carrying capacity-based normalisation in LCA: framework and development of references at midpoint level. Int. J. Life Cycle Assess. 20, 1005–1018. doi:10.1007/s11367-015-0899-2.

Bjørn, A., Owsianiak, M., Molin, C., Hauschild, M., 2018. LCA History, in: Life Cycle Assessment - Theory and Practice. Springer International Publishing.

Bjørn, A., Richardson, K., Hauschild, M.Z., 2019. A Framework for Development and Communication of Absolute Environmental Sustainability Assessment Methods. J. Ind. Ecol. 23, 838–854. doi:10.1111/jiec.12820.

Boas, I., Farbotko, C., Adams, H., Sterly, H., Bush, S., van der Geest, K., Wiegel, H., Ashraf, H., Baldwin, A., Bettini, G., Blondin, S., de Bruijn, M., Durand-Delacre, D., Fröhlich, C., Gioli, G., Guaita, L., Hut, E., Jarawura, F.X., Lamers, M., Lietaer, S., Nash, S.L., Piguet, E., Rothe, D., Sakdapolrak, P., Smith, L., Tripathy Furlong, B., Turhan, E., Warner, J., Zickgraf, C., Black, R., Hulme, M., 2019. Climate migration myths. Nat. Clim. Chang. 912 (9), 901–903. doi:10.1038/s41558-019-0633-3.

Brown, Thomas, Hörsch, J., Schlachtberger, D., 2018. PyPSA: Python for Power System Analysis. J. Open Res. Softw. 6, 4. doi:10.5334/JORS.188.

Brown, T., Schlachtberger, D., Kies, A., Schramm, S., Greiner, M., 2018. Synergies of sector coupling and transmission reinforcement in a cost-optimised, highly renewable European energy system. Energy 160, 720–739. doi:10.1016/J.ENERGY.2018.06.222.

Bucchianico, S. Di, Cappelli, F., Di Bucchianico, S., 2021. Exploring the theoretical link between profitability and luxury emissions.

Bunsen, J., Berger, M., Finkbeiner, M., 2021. Planetary boundaries for water – A review. Ecol. Indic. 121, 107022. doi:10.1016/J.ECOLIND.2020.107022.

Bussieck, M.R., Meeraus, A., 2004. General Algebraic Modeling System (GAMS). Springer, Boston, MA doi:10.1007/978-1-4613-0215-5_8.

Cali, U., Kuzlu, M., Pipattanasomporn, M., Kempf, J., Bai, L., 2021. Optimization and Digitalization of Power Markets, in: Digitalization of Power Markets and Systems Using Energy Informatics. Springer International Publishing, Cham, pp. 217–232. doi:10.1007/978-3-030-83301-5_10.

Calvert, K., Mabee, W., 2015. More solar farms or more bioenergy crops? Mapping and assessing potential land-use conflicts among renewable energy technologies in eastern Ontario. Canada. Appl. Geogr. 56, 209–221. doi:10.1016/j.apgeog.2014.11.028.

CGN2010, 2015. EU NUTS 2 population density 2007 [WWW Document]. Wikipedia.

Chandrakumar, C., Mclaren, S.J., 2018. Exploring the Linkages Between the Environmental Sustainable Development Goals and Planetary Boundaries Using the DPSIR Impact Pathway Framework, in: Designing Sustainable Technologies, Products and Policies. Springer International Publishing, pp. 413–423. doi:10.1007/978-3-319-66981-6.

Chen, C., Yang, A., 2021. Power-to-methanol: The role of process flexibility in the integration of variable renewable energy into chemical production. Energy Convers. Manag. 228, 113673. doi:10.1016/J.ENCONMAN.2020.113673.

Cheng, J., Jiang, H., Jiao, X., -, al, Yang, L., Cormican, K., 2017. Holistic energy system modeling combining multi-objective optimization and life cycle assessment. Environ. Res. Lett. 12, 124005. doi:10.1088/1748-9326/AA914D.

Cherp, A., Jewell, J., Goldthau, A., 2011. Governing Global Energy: Systems, Transitions. Complexity. Glob. Policy 2, 75–88. doi:10.1111/J.1758-5899.2010.00059.X.

Child, M., Koskinen, O., Linnanen, L., Breyer, C., 2018. Sustainability guardrails for energy scenarios of the global energy transition. Renew. Sustain. Energy Rev. 91, 321–334. doi:10.1016/J.RSER.2018.03.079.

Ciroth, A., Muller, S., Weidema, B., Lesage, P., 2016. Empirically based uncertainty factors for the pedigree matrix in ecoinvent. Int. J. Life Cycle Assess. 21, 1338–1348. doi:10.1007/s11367-013-0670-5.

Clarke, B.J., E.L. Otto, F., Jones, R.G., 2021. Inventories of extreme weather events and impacts: Implications for loss and damage from and adaptation to climate extremes. Clim. Risk Manag. 32, 100285. doi:10.1016/J.CRM.2021.100285.

Cranston, G., Steffen, W., 2019. Linking planetary boundaries to business.

Crespo del Granado, P., van Nieuwkoop, R.H., Kardakos, E.G., Schaffner, C., 2018. Modelling the energy transition: A nexus of energy system and economic models. Energy Strateg. Rev. 20, 229–235. doi:10.1016/J.ESR.2018.03.004.

Davis, S.J., Lewis, N.S., Shaner, M., Aggarwal, S., Arent, D., Azevedo, I.L., Benson, S.M., Bradley, T., Brouwer, J., Chiang, Y.-M., Clack, C.T.M., Cohen, A., Doig, S., Edmonds, J., Fennell, P., Field, C.B., Hannegan, B., Hodge, B.-M., Hoffert, M.I., Ingersoll, E., Jaramillo, P., Lackner, K.S., Mach, K.J., Mastrandrea, M., Ogden, J., Peterson, P.F., Sanchez, D.L., Sperling, D., Stagner, J., Trancik, J.E., Yang, C.-J., Caldeira, K., 2018. Net-zero emissions energy systems. Science (80-.) 360. doi:10.1126/SCIENCE.AAS9793.
De-León Almaraz, S., Azzaro-Pantel, C., Montastruc, L., Domenech, S., 2014. Hydrogen supply chain optimization for deployment scenarios in the Midi-Pyrénées region, France. Int. J. Hydrogen Energy 39, 11831–11845. doi:10.1016/J.IJHYDENE.2014.05.165.
de Baan, L., Mutel, C.L., Curran, M., Hellweg, S., Koellner, T., 2013. Land use in life cycle assessment: global characterization factors based on regional and global potential species extinction. Environ. Sci. Technol. 47, 9281–9290. doi:10.1021/es400592q.
Ehrenstein, M., Galán-Martín, Á., Tulus, V., Guillén-Gosálbez, G., 2020. Optimising fuel supply chains within planetary boundaries: A case study of hydrogen for road transport in the UK. Appl. Energy 276, 115486. doi:10.1016/j.apenergy.2020.115486.
GmbH, Energie-Atlas, 2005. Solar Energy in EUROPE [WWW Document]. Glob. Energy Netw. Inst.
Fanning, A.L., O'Neill, D.W., Hickel, J., Roux, N., 2021. The social shortfall and ecological overshoot of nations. Nat. Sustain. 2021, 1–11. doi:10.1038/s41893-021-00799-z.
Fathima, A.H., Palanisamy, K., 2015. Optimization in microgrids with hybrid energy systems – A review. Renew. Sustain. Energy Rev. 45, 431–446. doi:10.1016/J.RSER.2015.01.059.
FICO, 2018. FICO Xpress Optimization Reference Manual V33.01.
Fourer, R., Gay, D., Kernighan, B., 2003. AMPL. A modeling language for mathematical programming.
Freidberg, S., 2015. From behind the curtain: talking about values in LCA. Int. J. Life Cycle Assess. 237 (23), 1410–1414. doi:10.1007/S11367-015-0879-6.
Freire Ordóñez, D., Shah, N., Guillén-Gosálbez, G., 2021. Economic and full environmental assessment of electrofuels via electrolysis and co-electrolysis considering externalities. Appl. Energy 286, 116488. doi:10.1016/J.APENERGY.2021.116488.
Galán-Martín, A., Pozo, C., Azapagic, A., Grossmann, I.E., Dowell, N.Mac, Guillén-Gosálbez, G., 2018. Time for global action: an optimised cooperative approach towards effective climate change mitigation. Energy Environ. Sci. 11, 572–581. doi:10.1039/C7EE02278F.
Galán-Martín, Á., Vázquez, D., Cobo, S., Mac Dowell, N., Caballero, J.A., Guillén-Gosálbez, G., 2021. Delaying carbon dioxide removal in the European Union puts climate targets at risk. Nat. Commun. 2021 121 (12), 1–12. doi:10.1038/s41467-021-26680-3.
Galan-Martın, A., Tulus, V., Dıaz, I., Pozo, C., Perez-Ramırez, J., Guillen-Gosalbez, G., 2021. Sustainability footprints of a renewable carbon transition for the petrochemical sector within planetary boundaries. One Earth 4, 565–583. doi:10.1016/j.oneear.2021.04.001.
Garcia, D., You, F., 2018. Methods for Quantitative Consideration of Ecosystem Services in Supply Chain Design and Optimization. AIChE.
Ghosh, T., Bakshi, B.R., 2019. Designing biofuel supply chains while mitigating harmful algal blooms with treatment wetlands. Comput. Chem. Eng. 126, 113–127. doi:10.1016/j.compchemeng.2019.03.041.
Groen, E.A., Bokkers, E.A.M., Heijungs, R., de Boer, I.J.M., 2017. Methods for global sensitivity analysis in life cycle assessment. Int. J. Life Cycle Assess. 22, 1125–1137. doi:10.1007/s11367-016-1217-3.
Guillen-Gosalbez, G., Caballero, J.A., Esteller, L.J., Gadalla, M., 2007. Application of life cycle assessment to the structural optimization of process flowsheets. Comput. Aided Chem. Eng. 24, 1163–1168. doi:10.1016/S1570-7946(07)80218-5.
Guillén-Gosálbez, G., You, F., Galán-Martín, Á., Pozo, C., Grossmann, I.E., 2019. Process systems engineering thinking and tools applied to sustainability problems: current landscape and future opportunities. Curr. Opin. Chem. Eng. 26, 170–179. doi:10.1016/J.COCHE.2019.11.002.
Guinée, J.B., Koning, A., Heijungs, R., 2022. Life cycle assessment-based Absolute Environmental Sustainability Assessment is also relative. J. Ind. Ecol. 1–10. doi:10.1111/jiec.13260.
Gurobi Optimization, 2021. Gurobi Optimizer Reference Manual.
Hall, L.M.H., Buckley, A.R., 2016. A review of energy systems models in the UK: Prevalent usage and categorisation. Appl. Energy 169, 607–628. doi:10.1016/J.APENERGY.2016.02.044.
Hammond, G.P., Jones, C.I., O'Grady, Á., 2015. Environmental Life Cycle Assessment (LCA) of Energy Systems. Handb. Clean Energy Syst. 1–26. doi:10.1002/9781118991978.HCES139.
Hanafiah, M.M., Hendriks, A.J., Huijbregts, M.A.J., 2012. Comparing the ecological footprint with the biodiversity footprint of products. J. Clean. Prod. 37, 107–114. doi:10.1016/j.jclepro.2012.06.016.
Hare, B., Brecha, R., Schaeffer, M., 2018. Integrated Assessment Models: what are they and how do they arrive at their conclusions? [WWW Document]. Clim. Anal. IAMs Brief..
Hauschild, M.Z., Huijbregts, M.A.J., 2015. Introducing Life Cycle Impact Assessment. In: Hauschild, M.Z., Huijbregts, M.A.J. (Eds.), Life Cycle Impact Assessment, LCA Compendium—The Complete World of Life Cycle Assessment. Springer-Science+Business Media, BV, Dordrecht, pp. 1–16.
Hauschild, M.Z., Kara, S., Røpke, I., 2020. Absolute sustainability: Challenges to life cycle engineering. CIRP Ann 69, 533–553. doi:10.1016/j.cirp.2020.05.004.
Hauschild, M.Z., Rosenbaum, R.K., Olsen, S.I., 2018. Life cycle assessment, Life Cycle Assessment: Theory and Practice. Springer International Publishing, Cham doi:10.1007/978-3-319-56475-3.
Häyhä, T., Lucas, P.L., van Vuuren, D.P., Cornell, S.E., Hoff, H., 2016. From Planetary Boundaries to national fair shares of the global safe operating space — How can the scales be bridged? Glob. Environ. Chang. 40, 60–72. doi:10.1016/j.gloenvcha.2016.06.008.
Heijungs, R., 1995. Harmonization of methods for impact assessment. Environ. Sci. Pollut. Res. 2, 217–224. doi:10.1007/BF02986769.
Herbst, A., Toro, F., Reitze, F., Jochem, E., 2012. Introduction to Energy Systems Modelling. Statistics (Ber) 148, 111–135.
Hertwich, E.G., Wood, R., 2018. The growing importance of scope 3 greenhouse gas emissions from industry. Environ. Res. Lett. 13, 104013. doi:10.1088/1748-9326/AAE19A.
Hollberg, A., Kiss, B., Röck, M., Soust-Verdaguer, B., Wiberg, A.H., Lasvaux, S., Galimshina, A., Habert, G., 2021. Review of visualising LCA results in the design process of buildings. Build. Environ. 190, 107530. doi:10.1016/j.buildenv.2020.107530.
Howells, M., Rogner, H., Strachan, N., Heaps, C., Huntington, H., Kypreos, S., Hughes, A., Silveira, S., DeCarolis, J., Bazillian, M., Roehrl, A., 2011. OSeMOSYS: The Open Source Energy Modeling System: An introduction to its ethos, structure and development. Energy Policy 39, 5850–5870. doi:10.1016/J.ENPOL.2011.06.033.
Huang, L., Rao, C., van der Kuijp, T.J., Bi, J., Liu, Y., 2017. A comparison of individual exposure, perception, and acceptable levels of PM2.5 with air pollution policy objectives in China. Environ. Res. 157, 78–86. doi:10.1016/J.ENVRES.2017.05.012.
Huckebrink, D., Bertsch, V., 2021. Integrating Behavioural Aspects in Energy System Modelling—A Review. Energies 14, 4579. doi:10.3390/EN14154579.
Huppmann, D., Gidden, M., Fricko, O., Kolp, P., Orthofer, C., Pimmer, M., Kushin, N., Vinca, A., Mastrucci, A., Riahi, K., Krey, V., 2019. The MESSAGE ix Integrated Assessment Model and the ix modeling platform (ixmp). Environ. Model. Softw. 112, 143–156. doi:10.1016/j.envsoft.2018.11.012.
IBM, 2017. IBM ILOG CPLEX Optimization Studio CPLEX User's Manual V12.8.
ISO, 2006. Environmental management - Life cycle assessment - Principles and framework. ISO, Geneva.
James, R., Otto, F., Parker, H., Boyd, E., Cornforth, R., Mitchell, D., Allen, M., 2014. Characterizing loss and damage from climate change. Nat. Clim. Chang. 411 (4), 938–939. doi:10.1038/nclimate2411.
Keramidas, K., Kitous, A., Schmitz, J., 2017. POLES-JRC model documentation. doi:10.2760/225347.
Khan, F., 2019. Staying within planetary boundaries. Nat. Energy 44 (4), 260. doi:10.1038/s41560-019-0380-8.
Klemeš, J.J., Kravanja, Z., 2013. Forty years of Heat Integration: Pinch Analysis (PA) and Mathematical Programming (MP). Curr. Opin. Chem. Eng. 2, 461–474. doi:10.1016/J.COCHE.2013.10.003.
Komusanac, I., Brindley, G., Fraile, D., 2020. Wind energy in Europe in 2019. Brussels.
Lade, S.J., Steffen, W., Vries, W. De, Carpenter, S.R., Donges, J.F., Gerten, D., Hoff, H., Newbold, T., Richardson, K., Rockström, J., n.d. Human impacts on planetary boundaries amplified by Earth system interactions. doi:10.1038/s41893-019-0454-4.
Laurent, A., Espinosa, N., Hauschild, M.Z., 2018. LCA of Energy Systems. Life Cycle Assess. Theory Pract 633–668. doi:10.1007/978-3-319-56475-3_26.
Lesage, P., Mutel, C., Schenker, U., Margni, M., 2018. Uncertainty analysis in LCA using precalculated aggregated datasets. Int. J. Life Cycle Assess. 23, 2248–2265. doi:10.1007/S11367-018-1444-X/TABLES/6.
Leung Pah Hang, M.Y., Martinez-Hernandez, E., Leach, M., Yang, A., 2016. Designing integrated local production systems: A study on the food-energy-water nexus. J. Clean. Prod. 135, 1065–1084. doi:10.1016/j.jclepro.2016.06.194.
Li, M., Wiedmann, T., Fang, K., Hadjikakou, M., 2021. The role of planetary boundaries in assessing absolute environmental sustainability across scales. Environ. Int. 152, 106475. doi:10.1016/J.ENVINT.2021.106475.
Loulou, R., Labriet, M., 2007. ETSAP-TIAM: the TIMES integrated assessment model Part I: Model structure. Comput. Manag. Sci. 51 (5), 7–40. doi:10.1007/S10287-007-0046-Z.
Luderer, G., Leimbach, M., Bauer, N., Kriegler, E., Baumstark, Lavinia Bertram, C., Giannousakis, A., Hilaire, J., Klein, D., Levesque, A., Mouratiadou, I., Pehl, M., Pietzcker, R., Piontek, F., Roming, N., Schultes, A., Valeria Jana Schwanitz, J.S., 2015. Description of the REMIND Model (Version 1.6).
Luderer, G., Pehl, M., Arvesen, A., Gibon, T., Bodirsky, B.L., Sytze De Boer, H., Fricko, O., Hejazi, M., Humpenöder, F., Iyer, G., Mima, S., Mouratiadou, I., Pietzcker, R.C., Popp, A., Van Den Berg, M., Van Vuuren, D., Hertwich, E.G., 2019. Environmental co-benefits and adverse side-effects of alternative power sector decarbonization strategies. Nat. Commun. 10. doi:10.1038/s41467-019-13067-8.
Martín, M., Grossmann, I.E., 2017. Optimal integration of a self sustained algae based facility with solar and/or wind energy. J. Clean. Prod. 145, 336–347. doi:10.1016/J.JCLEPRO.2017.01.051.
McCollum, D.L., Zhou, W., Bertram, C., de Boer, H.-S., Bosetti, V., Busch, S., Després, J., Drouet, L., Emmerling, J., Fay, M., Fricko, O., Fujimori, S., Gidden, M., Harmsen, M., Huppmann, D., Iyer, G., Krey, V., Kriegler, E., Nicolas, C., Pachauri, S., Parkinson, S., Poblete-Cazenave, M., Rafaj, P., Rao, N., Rozenberg, J., Schmitz, A., Schoepp, W., Vuuren, D., van, Riahi, K., 2018. Energy investment needs for fulfilling the Paris Agreement and achieving the Sustainable Development Goals. Nat. Energy 37 (3), 589–599. doi:10.1038/s41560-018-0179-z.
Mendoza Beltran, A., Cox, B., Mutel, C., van Vuuren, D.P., Font Vivanco, D., Deetman, S., Edelenbosch, O.Y., Guinée, J., Tukker, A., 2020. When the Background

Matters: Using Scenarios from Integrated Assessment Models in Prospective Life Cycle Assessment. J. Ind. Ecol. 24, 64–79. doi:10.1111/JIEC.12825.
Montoya, J.M., Donohue, I., Pimm, S.L., 2018. Planetary Boundaries for Biodiversity: Implausible Science, Pernicious Policies. Trends Ecol. Evol. 33, 71–73. doi:10.1016/J.TREE.2017.10.004.
Moomen, A.W., Dewan, A., 2017. Probing the Perspectives of Stakeholder Engagement and Resistance Against Large-Scale Surface Mining in Developing Countries. Corp. Soc. Responsib. Environ. Manag. 24, 85–95. doi:10.1002/CSR.1396.
Muller, S., Mutel, C., Lesage, P., Samson, R., 2018. Effects of Distribution Choice on the Modeling of Life Cycle Inventory Uncertainty: An Assessment on the Ecoinvent v2.2 Database. J. Ind. Ecol. 22, 300–313. doi:10.1111/JIEC.12574.
Negri, V., Galán-Martín, Á., Pozo, C., Fajardy, M., Reiner, D.M., Mac Dowell, N., Guillén-Gosálbez, G., 2021. Life cycle optimization of BECCS supply chains in the European Union. Appl. Energy 298. doi:10.1016/j.apenergy.2021.117252.
O'Neill, D.W., Fanning, A.L., Lamb, W.F., Steinberger, J.K., Neill, D.W.O., Fanning, A.L., Lamb, W.F., Steinberger, J.K., 2018. A good life for all within planetary boundaries. Nat. Sustain. 1, 88–95. doi:10.1038/s41893-018-0021-4.
Ogumerem, G.S., Tso, W.W., Demirhan, C.D., Lee, S.Y., Song, H.E., Pistikopoulos, E.N., 2019. Toward the Optimization of Hydrogen, Ammonia, and Methanol Supply Chains. IFAC-PapersOnLine 52, 844–849. doi:10.1016/J.IFACOL.2019.06.167.
Pehl, M., Arvesen, A., Humpenöder, F., Popp, A., Hertwich, E.G., Luderer, G., 2017. Understanding future emissions from low-carbon power systems by integration of life-cycle assessment and integrated energy modelling. Nat. Energy. doi:10.1038/s41560-017-0032-9.
Pennington, D.W., Potting, J., Finnveden, G., Lindeijer, E., Jolliet, O., Rydberg, T., Rebitzer, G., 2004. Life cycle assessment Part 2: Current impact assessment practice. Environ. Int. 30, 721–739. doi:10.1016/J.ENVINT.2003.12.009.
Persson, L., Carney Almroth, B.M., Collins, C.D., Cornell, S., de Wit, C.A., Diamond, M.L., Fantke, P., Hassellöv, M., MacLeod, M., Ryberg, M.W., Søgaard Jørgensen, P., Villarrubia-Gómez, P., Wang, Z., Hauschild, M.Z., 2022. Outside the Safe Operating Space of the Planetary Boundary for Novel Entities. Environ. Sci. Technol. doi:10.1021/acs.est.1c04158.
Pfenninger, S., 2017. Energy scientists must show their workings. Nat. 2017 5427642 542, 393. doi:10.1038/542393a.
Pfenninger, S., DeCarolis, J., Hirth, L., Quoilin, S., Staffell, I., 2017. The importance of open data and software: Is energy research lagging behind? Energy Policy 101, 211–215. doi:10.1016/J.ENPOL.2016.11.046.
Pfister, S., Ridoutt, B., 2015. Proposed planetary boundary for freshwater sends a dangerous message. doi:10.13140/RG.2.2.11939.78882.
Pieragostini, C., Mussati, M.C., Aguirre, P., 2012. On process optimization considering LCA methodology. J. Environ. Manage. 96, 43–54. doi:10.1016/J.JENVMAN.2011.10.014.
Pörtner, H.O., Scholes, R.J., Agard, J., Archer, E., Arneth, A., Bai, X., Barnes, D., Burrows, M., Chan, L., Cheung, W.L., Diamond, S., Donatti, C., Duarte, C., Eisenhauer, N., Foden, W., Gasalla, M., Handa, C., Hickler, T., Hoegh-Guldberg, O., Ichii, K., Jacob, U., Insarov, G., Kiessling, W., Leadley, P., Leemans, R., Levin, L., Lim, M., Maharaj, S., Managi, S., Marquet, P., McElwee, P., Midgley, G., Oberdorff, T., Obura, D., Osman, E., Pandit, R., Pascual, U., Pires, A.P.F., Popp, A., Reyes-García, V., Sankaran, M., Settele, J., Shin, Y.J., Sintayehu, D.W., Smith, P., Steiner, N., Strassburg, B., Sukumar, R., Trisos, C., Val, A.L., Wu, J., Aldrian, E., Parmesan, C., Pichs-Madruga, R., Roberts, D.C., Rogers, A., Díaz, S., Fischer, M., Hashimoto, S., Lavorel, S., Wu, N., Ngo, H.T., 2021. IPBES-IPCC co-sponsored workshop report on biodiversity and climate change. Intergovernmental Science-Policy Platform on Biodiversity and Ecosystem Services (IPBES) and Intergovernmental Panel on Climate Change (IPCC) https://doi.org/10.2/JQUERY.MIN.JS.
Rambhujun, N., Salman, M.S., Wang, T., Pratthana, C., Sapkota, P., Costalin, M., Lai, Q., Aguey-Zinsou, K.-F., 2020. Renewable hydrogen for the chemical industry. MRS Energy Sustain 7. doi:10.1557/MRE.2020.33.
Randers, J., Rockström, J., Stoknes, P., Goluke, U., Collste, D., Cornell, S.E., Donges, J., 2019. Achieving the 17 Sustainable Development Goals within 9 planetary boundaries. Glob. Sustain. 2, 1–11. doi:10.1017/sus.2019.22.
Raworth, K., 2017. A Doughnut for the Anthropocene: humanity's compass in the 21st century. Lancet Planet. Heal. 1, e48–e49. doi:10.1016/S2542-5196(17)30028-1.
Rebitzer, G., Ekvall, T., Frischknecht, R., Hunkeler, D., Norris, G., Rydberg, T., Schmidt, W.P., Suh, S., Weidema, B.P., Pennington, D.W., 2004. Life cycle assessment: Part 1: Framework, goal and scope definition, inventory analysis, and applications. Environ. Int. 30, 701–720. doi:10.1016/J.ENVINT.2003.11.005.
Riahi, K., van Vuuren, D.P., Kriegler, E., Edmonds, J., O'Neill, B.C., Fujimori, S., Bauer, N., Calvin, K., Dellink, R., Fricko, O., Lutz, W., Popp, A., Cuaresma, J.C., KC, S., Leimbach, M., Jiang, L., Kram, T., Rao, S., Emmerling, J., Ebi, K., Hasegawa, T., Havlik, P., Humpenöder, F., Da Silva, L.A., Smith, S., Stehfest, E., Bosetti, V., Eom, J., Gernaat, D., Masui, T., Rogelj, J., Strefler, J., Drouet, L., Krey, V., Luderer, G., Harmsen, M., Takahashi, K., Baumstark, L., Doelman, J.C., Kainuma, M., Klimont, Z., Marangoni, G., Lotze-Campen, H., Obersteiner, M., Tabeau, A., Tavoni, M., 2017. The Shared Socioeconomic Pathways and their energy, land use, and greenhouse gas emissions implications: An overview. Glob. Environ. Chang. 42, 153–168. doi:10.1016/J.GLOENVCHA.2016.05.009.
Ringkjøb, H.K., Haugan, P.M., Solbrekke, I.M., 2018. A review of modelling tools for energy and electricity systems with large shares of variable renewables. Renew. Sustain. Energy Rev. 96, 440–459. doi:10.1016/J.RSER.2018.08.002.
Ritchie, H., Roser, M., 2020. CO_2 and Greenhouse Gas Emissions [WWW Document]. Our World Data.
Rockström, J., Gupta, J., Lenton, T.M., Qin, D., Lade, S.J., Abrams, J.F., Jacobson, L., Rocha, J.C., Zimm, C., Bai, X., Bala, G., Bringezu, S., Broadgate, W., Bunn, S.E., DeClerck, F., Ebi, K.L., Gong, P., Gordon, C., Kanie, N., Liverman, D.M., Nakicenovic, N., Obura, D., Ramanathan, V., Verburg, P.H., van Vuuren, D.P., Winkelmann, R., 2021. Identifying a Safe and Just Corridor for People and the Planet. Earth's Futur 9, 1–7. doi:10.1029/2020EF001866.
Rockström, J., Steffen, W., Noone, K., Persson, Å., Chapin, F.S., Lambin, E., Lenton, T.M., Scheffer, M., Folke, C., Schellnhuber, H.J., Nykvist, B., de Wit, C.A., Hughes, T., van der Leeuw, S., Rodhe, H., Sörlin, S., Snyder, P.K., Costanza, R., Svedin, U., Falkenmark, M., Karlberg, L., Corell, R.W., Fabry, V.J., Hansen, J., Walker, B., Liverman, D., Richardson, K., Crutzen, P., Foley, J., 2009. Planetary boundaries: Exploring the safe operating space for humanity. Ecol. Soc. 14. doi:10.5751/ES-03180-140232.
Rugani, B., Maia de Souza, D., Weidema, B.P., Bare, J., Bakshi, B., Grann, B., Johnston, J.M., Pavan, A.L.R., Liu, X., Laurent, A., Verones, F., 2019. Towards integrating the ecosystem services cascade framework within the Life Cycle Assessment (LCA) cause-effect methodology. Sci. Total Environ. 690, 1284–1298. doi:10.1016/j.scitotenv.2019.07.023.
Ryberg, M.W., Andersen, M.M., Owsianiak, M., Hauschild, M.Z., 2020. Downscaling the planetary boundaries in absolute environmental sustainability assessments – A review. J. Clean. Prod. 276, 123287. doi:10.1016/j.jclepro.2020.123287.
Ryberg, M.W., Bjerre, T.K., Nielsen, P.H., Hauschild, M., 2021. Absolute environmental sustainability assessment of a Danish utility company relative to the Planetary Boundaries. J. Ind. Ecol. 25, 765–777. doi:10.1111/JIEC.13075.
Ryberg, Morten Walbech, Owsianiak, M., Clavreul, J., Mueller, C., Sim, S., King, H., Hauschild, M.Z., 2018a. How to bring absolute sustainability into decision-making: An industry case study using a Planetary Boundary-based methodology. Sci. Total Environ. 634, 1406–1416. doi:10.1016/j.scitotenv.2018.04.075.
Ryberg, Morten Walbech, Owsianiak, M., Richardson, K., Hauschild, M.Z., 2018b. Development of a life-cycle impact assessment methodology linked to the Planetary Boundaries framework. Ecol. Indic. 88, 250–262. doi:10.1016/j.ecolind.2017.12.065.
Ryberg, M.W., Owsianiak, M., Richardson, K., Hauschild, M.Z., 2016. Challenges in implementing a Planetary Boundaries based Life-Cycle Impact Assessment Methodology. J. Clean. Prod. 139, 450–459. doi:10.1016/j.jclepro.2016.08.074.
Sacchi, R., Terlouw, T., Siala, K., Bauer, C., Cox, B., Daioglou, V., Luderer, G., 2021. Prospective Environmental Impact Assesment (premise): a streamlined approach to producing databases for prospective Life Cycle Assessment using Integrated Assessment Models. Renew. Sustain. Energy Rev..
Sala, S., Andreasson, J., 2018. Improving interpretation, presentation and visualisation of LCA studies for decision making support, in: Designing Sustainable Technologies, Products and Policies. Springer, pp. 337–342.
Sala, S., Crenna, E., Secchi, M., Sanyé-Mengual, E., 2020. Environmental sustainability of European production and consumption assessed against planetary boundaries. J. Environ. Manage. 269. doi:10.1016/j.jenvman.2020.110686.
Sandin, G., Peters, G.M., Svanström, M., 2015. Using the planetary boundaries framework for setting impact-reduction targets in LCA contexts. Int. J. Life Cycle Assess. 20, 1684–1700. doi:10.1007/s11367-015-0984-6.
Schiffer, Z.J., Manthiram, K., 2017. Electrification and Decarbonization of the Chemical Industry. Joule 1, 10–14. doi:10.1016/J.JOULE.2017.07.008.
Scholz, Y., Fuchs, B., Borggrefe, F., Cao, K.-K., Wetzel, M., Von Krbek, K., Cebulla, F., Gils, H.C., Fiand, F., Bussieck, M., Koch, T., Rehfeldt, D., Gleixner, A., Khabi, D., Breuer, T., Rohe, D., Hobbie, H., Schönheit, D., Hasan¨, H., Yilmaz, H., Panos, E., Jeddi, S., Buchholz, S., 2020. Speeding up Energy System Models-a Best Practice Guide.
Stadler, K., Wood, R., Bulavskaya, T., Södersten, C.J., Simas, M., Schmidt, S., Usubiaga, A., Acosta-Fernández, J., Kuenen, J., Bruckner, M., Giljum, S., Lutter, S., Merciai, S., Schmidt, J.H., Theurl, M.C., Plutzar, C., Kastner, T., Eisenmenger, N., Erb, K.H., de Koning, A., Tukker, A., 2018. EXIOBASE 3: Developing a Time Series of Detailed Environmentally Extended Multi-Regional Input-Output Tables. J. Ind. Ecol. 00. doi:10.1111/jiec.12715.
Steffen, W., Richardson, K., Rockström, J., Cornell, S.E., Fetzer, I., Bennett, E.M., Biggs, R., Carpenter, S.R., de Vries, W., de Wit, C.A., Folke, C., Gerten, D., Heinke, J., Mace, G.M., Persson, L.M., Ramanathan, V., Reyers, B., Sorlin, S., 2015. Planetary boundaries: Guiding human development on a changing planet. Science (80-.) 347, 736. doi:10.1126/science.1259855.
Stehfest, E., van Vuuren, D., Bouwman, L., Kram, T., 2014. Integrated assessment of global environmental change with IMAGE 3.0: Model description and policy applications. Netherlands Environmental Assessment Agency.
Stern, N., 2013. The Structure of Economic Modeling of the Potential Impacts of Climate Change: Grafting Gross Underestimation of Risk onto Already Narrow Science Models. J. Econ. Lit. 51, 838–859. doi:10.1257/JEL.51.3.838.
Sterner, T., Barbier, E.B., Bateman, I., van den Bijgaart, I., Crépin, A.-S., Edenhofer, O., Fischer, C., Habla, W., Hassler, J., Johansson-Stenman, O., Lange, A., Polasky, S., Rockström, J., Smith, H.G., Steffen, W., Wagner, G., Wilen, J.E., Alpízar, F., Azar, C., Carless, D., Chávez, C., Coria, J., Engström, G., Jagers, S.C., Köhlin, G., Löfgren, Å., Pleijel, H., Robinson, A., 2019. Policy design for the Anthropocene. Nat. Sustain. 2, 14–21. doi:10.1038/s41893-018-0194-x.
Steubing, B., de Koning, D., Haas, A., Mutel, C.L., 2020. The Activity Browser — An open source LCA software building on top of the brightway framework. Softw. Impacts 3, 100012. doi:10.1016/j.simpa.2019.100012.
Subramanian, A.S.R., Gundersen, T., Adams, T.A., 2018. Modeling and Simulation of Energy Systems: A Review. Process 6, 238. doi:10.3390/PR6120238.
Thomsen, J., Hussein, N.S., Dolderer, A., Kost, C., 2021. Effect of the Foresight Horizon on Computation Time and Results Using a Regional Energy Systems Optimization Model. Energies 14, 495. doi:10.3390/EN14020495.

Tonini, Davide, Astrup, Thomas, 2012. LCA of biomass-based energy systems: A case study for Denmark. Applied Energy 99, 234–246. doi:10.1016/J.APENERGY.2012.03.006.

Trabucco, Antonio;, Zomer, R., 2019. Global Aridity Index and Potential Evapotranspiration (ET0) Climate Database v2. figshare. Fileset. doi:10.6084/m9.figshare.7504448.v3.

Treyer, K., Bauer, C., 2016. Life cycle inventories of electricity generation and power supply in version 3 of the ecoinvent database—part I: electricity generation. Int. J. Life Cycle Assess. 21, 1236–1254. doi:10.1007/S11367-013-0665-2/TABLES/7.

Tröndle, T., Lilliestam, J., Marelli, S., Pfenninger, S., 2020. Trade-Offs between Geographic Scale, Cost, and Infrastructure Requirements for Fully Renewable Electricity in Europe. Joule 4, 1929–1948. doi:10.1016/J.JOULE.2020.07.018.

Valente, Antonio, Tulus, Victor, Galán-Martín, Ángel, Huijbregts, J., Gonzalo Guillén-Gosálbez, M.A., 2021. The role of hydrogen in heavy transport to operate within planetary boundaries. Sustain. Energy Fuels 5, 4637–4649. doi:10.1039/D1SE00790D.

van Oldenborgh, G.J., van der Wiel, K., Kew, S., Philip, S., Otto, F., Vautard, R., King, A., Lott, F., Arrighi, J., Singh, R., van Aalst, M., 2021. Pathways and pitfalls in extreme event attribution. Clim. Chang. 2021 1661 166, 1–27. doi:10.1007/S10584-021-03071-7.

Vandepaer, L., Treyer, K., Mutel, C., Bauer, C., Amor, B., 2019. The integration of long-term marginal electricity supply mixes in the ecoinvent consequential database version 3.4 and examination of modeling choices. Int. J. Life Cycle Assess. 24, 1409–1428. doi:10.1007/S11367-018-1571-4/FIGURES/6.

Vargas-Gonzalez, M., Witte, F., Martz, P., Gilbert, L., Humbert, S., Jolliet, O., van Zelm, R., L'Haridon, J., 2019. Operational Life Cycle Impact Assessment weighting factors based on Planetary Boundaries: Applied to cosmetic products. Ecol. Indic. 107, 105498. doi:10.1016/j.ecolind.2019.105498.

Vargas, L., Willemen, L., Hein, L., 2017. Linking planetary boundaries and ecosystem accounting, with an illustration for the Colombian Orinoco river basin. Reg. Environ. Chang. 18, 1521–1534. doi:10.1007/s10113-018-1282-1.

Vázquez, D., Guillén-Gosálbez, G., 2021. Process design within planetary boundaries: Application to CO2 based methanol production. Chem. Eng. Sci. 246, 116891. doi:10.1016/J.CES.2021.116891.

Verones, F., Hellweg, S., Antón, A., Azevedo, L.B., Chaudhary, A., Cosme, N., Cucurachi, S., de Baan, L., Dong, Y., Fantke, P., Golsteijn, L., Hauschild, M., Heijungs, R., Jolliet, O., Juraske, R., Larsen, H., Laurent, A., Mutel, C.L., Margni, M., Núñez, M., Owsianiak, M., Pfister, S., Ponsioen, T., Preiss, P., Rosenbaum, R.K., Roy, P.O., Sala, S., Steinmann, Z., van Zelm, R., Van Dingenen, R., Vieira, M., Huijbregts, M.A.J., 2020. LC-IMPACT: A regionalized life cycle damage assessment method. J. Ind. Ecol. 24, 1201–1219. doi:10.1111/JIEC.13018.

Villarrubia-Gómez, P., Cornell, S.E., Fabres, J., 2018. Marine plastic pollution as a planetary boundary threat – The drifting piece in the sustainability puzzle. Mar. Policy 96, 213–220. doi:10.1016/j.marpol.2017.11.035.

Vohra, K., Vodonos, A., Schwartz, J., Marais, E.A., Sulprizio, M.P., Mickley, L.J., 2021. Global mortality from outdoor fine particle pollution generated by fossil fuel combustion: Results from GEOS-Chem. Environ. Res. 195, 110754. doi:10.1016/J.ENVRES.2021.110754.

Volkart, K., Mutel, C.L., Panos, E., 2018. Integrating life cycle assessment and energy system modelling: Methodology and application to the world energy scenarios. Sustain. Prod. Consum. 16, 121–133. doi:10.1016/J.SPC.2018.07.001.

Volkart, K., Weidmann, N., Bauer, C., Hirschberg, S., 2017. Multi-criteria decision analysis of energy system transformation pathways: A case study for Switzerland. Energy Policy 106, 155–168. doi:10.1016/J.ENPOL.2017.03.026.

Wagener, T., Pianosi, F., 2019. What has Global Sensitivity Analysis ever done for us? A systematic review to support scientific advancement and to inform policy-making in earth system modelling. Earth-Science Rev 194, 1–18. doi:10.1016/J.EARSCIREV.2019.04.006.

Wheeler, J., Galán-Martín, Á., Mele, F.D., Guillén-Gosálbez, G., 2021. Designing biomass supply chains within planetary boundaries. AIChE J 67, 1–15. doi:10.1002/aic.17131.

Wheeler, J., Páez, M.A., Guillén-Gosálbez, G., Mele, F.D., 2018. Combining multi-attribute decision-making methods with multi-objective optimization in the design of biomass supply chains. Comput. Chem. Eng. 113, 11–31. doi:10.1016/J.COMPCHEMENG.2018.02.010.

Wu, Y., Su, D., 2020. Review of Life Cycle Impact Assessment (LCIA) Methods and Inventory Databases. In: Sustainable Product Development. Springer, Cham, pp. 39–55. doi:10.1007/978-3-030-39149-2_3.

Li, Yinan, Lan, Song, Pérez-Ramírez, Javier, Wang, Xiaonan, 2020. Achieving a low-carbon future through the energy–chemical nexus in China. Sustain. Energy Fuels 4, 6141–6155. doi:10.1039/D0SE01337D.

Yue, D., Pandya, S., You, F., 2016. Integrating Hybrid Life Cycle Assessment with Multiobjective Optimization: A Modeling Framework. Environ. Sci. Technol. 50, 1501–1509. doi:10.1021/acs.est.5b04279.

Zhang, Q., Grossmann, I.E., Lima, R.M., 2016. On the relation between flexibility analysis and robust optimization for linear systems. AIChE J 62, 3109–3123. doi:10.1002/AIC.15221.

Zhu, K., Victoria, M., Brown, T., Andresen, G.B., Greiner, M., 2019. Impact of CO2 prices on the design of a highly decarbonised coupled electricity and heating system in. Europe. Appl. Energy 236, 622–634. doi:10.1016/J.APENERGY.2018.12.016.