Supplementary Materials

1. Place of Criteria in the Identification Key

Table 1 contains an overview of the criteria found in literature and a discussion per criteria in which domain of the sustainability assessment identification key they belong.

Table S1. Criteria found in literature on method selection and explanation on position in Identification Key.

Criteria	Explanation why in this domain	References
Domain: System boundaries/Inventory		
Object	Methods are often specialised for a specific type of object. Many methods are flexible in this sense, with adjustments they can be applied to other subjects. Still, we think the object is a leading criteria in method selection. The object determines the type of inventory that is required. It is not a key criteria for Impact assessment/Theme selection. For example, a theme like toxic pressure by the use of pesticides can be a relevant theme for any type of object: a product, a farm, agriculture as a sector and a region. The object is also not key for selection of the type of Aggregation/Interpretation required.	[1–6]
Spatial focus of the activity	Methods have clear restrictions in the spatial focus they are able to attend. Life cycle inventories focus on micro level, Cost Benefit Analysis (CBA) and input-output analyses on meso (organisation or sector) or macro level (economy wide), while risk assessment focusses on the local or regional level.	[1,3–7]
Temporal focus of the assessment	The temporal focus (retro-, present-, or prospective) determines the type of data, inventory, that is required. Many of the methods marked as retro- or present-spective by for example Ness *et al.* can be used in a prospective manner by using data from a scenario analysis instead of measurements from the past.	[3,4,8–10]
Life cycle thinking	Although in principle, working from a life cycle thinking perspective is not exclusive for Life Cycle Analysis (LCA), Life Cycle Costing (LCC) or Social-LCA, but can be applied within any methodology, it asks a lot from modelling and database perspective, therefor we see this criteria as key for selection of a method. The form of life cycle thinking applied does depend on the object and spatial focus of the assessment. Life cycle assessments can be performed on products and processes. For assessments on organisations or regions chain analysis make more sense.	[6,11,12]

Table S1. *Cont.*

Criteria	Explanation why in this domain	References
Domain: Impact Assessment/Theme selection		
What is to be sustained	The answer on the question what is to be sustained determines which themes are to be selected. Quantification of themes is not evenly developed for the different type of receptors (social, environmental, cultural, economic), in general there is more experience with quantification of environmental and economic indicators than with social and cultural indicators. Indirect, receptor focus can determine method selection via theme selection.	[3,4,7,9,13,14]
Theme and indicator selection	Which themes are selected does have an influence on the choice of method, because not every theme can be quantified with every methodology. The match between theme selection and method selection is performed at the end of the identification key and is therefore not part of one of the sub identification keys. However, what is part of the identification key are characteristics of the themes: is the focus on impacts or pressures *etc.*?	[2,5,6,13,15]
Spatial focus of impact	The focus of impact assessments can be either object specific, within the boundaries of the location where the activity takes place, or it can be broader, taking also into account impacts elsewhere caused by the activities. For example, toxic substances emitted in a region can "travel" and thus cause effects outside that region. Furthermore, to determine impacts two approaches exist: site dependent or site-independent impact estimation. The first determines the impact based on the characteristics of a given location, the latter determines the impact independent of where the activity takes place.	[1,6,9,12,15]
Temporal focus of the impact	To take into account impact on other generations is common practice for the environmental part of sustainability analysis. For example in some Life cycle impact assessment (LCIA) methods the characterisation factors with which pressures can be expressed as impacts depend on which cultural perspective is chosen, which come with a view on the temporal focus of the impacts (e.g., 20, 100 or 1000 years). The temporal focus of socio-economic impacts tend to be shorter than for environmental impacts.	[7,9,10,14,16]
Domain: Aggregation/Interpretation		
Sustainability target	Some method present the results intrinsically against a benchmark or sustainability target (e.g., ecological footprint), however in principle the results of every assessment can be held against sustainability targets.	[8–10,12]

Table S1. *Cont.*

Criteria	Explanation why in this domain	References
Domain: Aggregation/Interpretation		
Values/View on sustainability	One's view on sustainability determines how results are interpreted. E.g., from weak sustainability point of view impacts on the different capitals are interchangeable: e.g., gaining economic capital by losing social capital can be seen as sustainable, as long as the total capital stays the same (or increases). While from strong sustainability point of view, impacts on the different capitals are not interchangeable: the loss of one capital cannot be justified by gaining other capital. Thus, depending on one's view on sustainability, different conclusions can be drawn based on the same results (same indicators and quantification). Also, one's world view, the way people perceive risks *etc.* determine how results are interpreted. Therefore, this criteria belongs to the domain aggregation and interpretation. NB: other elements that could be seen as "view on sustainability", e.g., "what should be sustained", are covered by other criteria.	[5,8,10,14,16–22]
View on integration of pillars	Methodologies can be part of multi-, inter- or trans-disciplinary assessments. Multidisciplinary means that results from different disciplines are simultaneously presented; interdisciplinary means that results from different disciplines are aggregated somehow; and transdisciplinairy means that assessments are mingled and thus asks for methodology tuning or even new methodology development. In the theme selection phase, the view on disciplinarity can be taken into account, e.g., by choosing indicators that refer to different disciplines, or indicators of interaction between phenomena within different disciplines. Also, the procedure to select themes can have different forms: with our without interaction between disciplines. Combining quantification methods from different disciplines, might needs adjustment of these methods, e.g., to streamline the assumption like time horizon etcetera. Thus the type of integration determines how this step in aggregation is interwoven in the other domains.	[4,9–11,14,16]
Normalisation/weighting/ aggregation method	Evidently, the level of aggregation preferred determines the level of aggregation needed. The type of normalisation, weighting and aggregation is determined by the view on sustainability and perspective from which the assessment is performed, but also from the way indicators are quantified (e.g., if an arithmetic or geometric mean should be used).	[5–7,12–14,18]
Domain: Method Design		
View on stakeholder involvement	Participation of stakeholders can theoretically be imbedded in every assessment and thus method design.	[7,10,14,16,19,23,24]

Table S1. *Cont.*

Criteria	Explanation why in this domain	References
Context of the assessment	The phase in a procedure for which an assessment is needed, and the accompanied goal of the assessment (decision making, advocacy, research, *etc.*) determine how an assessment is performed and presented (quick scan or thoroughly examination; amount of details; *etc.*). Like Hacking *et al.* [9] we argue that most methodologies are flexible enough to play a role within different contexts and thus this is no key criteria. It rather defines the method design and presentation of the results.	[1–3,7,23]
Uncertainties	Uncertainty, sensitivity, perturbation assessments *etc.* can be added to any assessment.	[1,7,9,10,14,25]
Domain: Organisational restrictions		
Formal recognition	Some authors stipulate the importance for formal recognition of a methodology as a criteria for method selection. However, it is not yet clear what is and what is not formal recognition. E.g., is it important that it has an ISO standard, or is it important how much or by whom it is used? For now we exclude this criteria from the identification key.	[1,7]
Data requirements and availability	Although taken up in the conceptual model of this paper, these boundary conditions are not yet operationalized. For now we focus of the best suitable methodology, without taking into account organisational restrictions.	[1,7,12,26]
Software requirements and availability	Although taken up in the conceptual model of this paper, these boundary conditions are not yet operationalized. For now we focus of the best suitable methodology, without taking into account organisational restrictions.	[1,5]
Expertise requirements and availability	Although taken up in the conceptual model of this paper, these boundary conditions are not yet operationalized. For now we focus of the best suitable methodology, without taking into account organisational restrictions.	[1,5,14]

2. The Sustainability Assessment Identification Key

The first design of the sustainability assessment identification key for the domain "System Boundaries/Inventory" is provided as interactive pdf document as an example (Supporting Information part 2_011214.pdf). The key is operationalized with a selection of methods (27 different methods).

3. List of the 30 Selected Case Studies

Table S2. Selection of case studies from literature.

First Author	Year	Title	Reference
Bausch	2014	Agro-environmental sustainability assessment using multicriteria decision analysis and system analysis	[27]
Cissé	2014	Sustainability of tropical small-scale fisheries: Integrated assessment in French Guiana	[28]
Dombi	2014	Sustainability assessment of renewable power and heat generation technologies	[29]
Maxim	2014	Sustainability assessment of electricity generation technologies using weighted multi-criteria analysis	[30]
Park	2014	Quantitative Sustainability Assessment of Seaweed Biomass as Bioethanol Feedstock	[31]
Schernewski	2014	Application and evaluation of an indicator set to measure and promote sustainable development in coastal areas	[32]
Brown	2013	Sustainability assessment of renovation packages for increased energy efficiency for multi-family buildings in Sweden	[33]
Duarte	2013	Sustainability assessment of sugarcane-ethanol production in Brazil: A case study of a sugarcane mill in São Paulo state	[34]
Ibáñez-Forés	2013	Assessing the sustainability of Best Available Techniques (BAT): Methodology and application in the ceramic tiles industry	[35]
LeCorre	2013	Comparative Sustainability Assessment of Starch Nanocrystals	[36]
Luthe	2013	A systems approach to sustainable technical product design: Combining life cycle assessment and virtual development in the case of skis	[37]
Phillips	2013	Determining the sustainability of options for municipal solid waste disposal in Varanasi, India.	[38]
Riera Pérez	2013	A multi-criteria approach to compare urban renewal scenarios for an existing neighborhood. Case study in Lausanne (Switzerland)	[39]
Song	2013	Sustainability evaluation of e-waste treatment based on emergy analysis and the LCA method: A case study of a trial project in Macau	[40]
Binder	2012	Sustainability solution space of the Swiss milk value added chain	[41]
Castellani	2012	Ecological Footprint and Life Cycle Assessment in the sustainability assessment of tourism activities	[42]
Florin	2012	Selecting the sharpest tools to explore the food-feed-fuel debate: Sustainability assessment of family farmers producing food, feed and fuel in Brazil	[43]
Liu	2012	Sustainability assessment of bioethanol and petroleum fuel production in Japan based on emergy analysis	[44]
Mata	2012	LCA Tool for Sustainability Evaluations in the Pharmaceutical Industry	[45]
Nzila	2012	Multi criteria sustainability assessment of biogas production in Kenya	[46]

Table S2. *Cont.*

First Author	Year	Title	Reference
Oudshoorn	2012	Sustainability evaluation of automatic and conventional milking systems on organic dairy farms in Denmark	[47]
Silalertruksa	2012	Environmental sustainability assessment of palm biodiesel production in Thailand	[48]
Stamford	2012	Life cycle sustainability assessment of electricity options for the UK	[49]
Tatari	2012	Comparative sustainability assessment of warm-mix asphalts: A thermodynamic based hybrid life cycle analysis	[50]
Tokos	2012	An integrated sustainability performance assessment and benchmarking of breweries	[51]
Traverso	2012	Towards life cycle sustainability assessment: an implementation to photovoltaic modules	[52]
Van Passel	2012	Multilevel and multi-user sustainability assessment of farming systems	2 case studies: [53]
Vermeulen	2012	Sustainability assessment of industrial waste treatment processes: The case of automotive shredder residue	[54]
Corbire	2011	Towards a global criteria based framework for the sustainability assessment of bioethanol supply chains Application to the Swiss dilemma: Is local produced bioethanol more sustainable than bioethanol imported from Brazil?	[55]

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