Global Guidance on Environmental Life Cycle Impact Assessment Indicators

Volume 2

United Nations Environment Programme

Life Cycle Initiative

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Foreword - UN Environment

The official documents endorsed in the Fourth Session of the UN Environment Assembly (UNEA4), held in Nairobi from 11–15 March 2019, provide a strong acknowledgement that life cycle approaches (including Life Cycle Assessment, LCA) are a must to achieve sustainable consumption and production, increase resource efficiency, and reduce risks (e.g., of hazardous chemicals and all forms of waste). LCA is the most robust tool to provide the systems perspective required to accelerate the shift towards more sustainable consumption and production patterns. Life Cycle Assessment informs the footprint metrics that allow us to monitor whether we're shifting the needle of decoupling human prosperity from environmental impacts. These metrics enable the comparison between product systems, and the identification of the main hotspots driving impacts in such systems as well as of potential trade-offs among them. Indicators that clearly show the links between human interventions and environmental impacts (externalities) are needed. But the pathway from human interventions to such impacts can be complex, with numerous different indicators being used to capture results. This reduces the comparability between studies, limiting the definition of clear preferences between products and practices, as well as the usability of results.

The *Global Guidance for Life Cycle Impact Assessment Indicators 2* is continuation of a series of reports addressing these issues. Aimed at life cycle assessment practitioners and method developers, it identifies the "current best available practice" in a variety of areas. This 2nd Volume focuses on Acidification & Eutrophication, Human Toxicity and Ecotoxicity, Mineral Resources, and Soil Quality. The global importance of these impact areas is also recognized in specific Sustainable Development Goals (SDGs), as well as in several resolutions of UNEA4.

The guidance also strengthens the position of the Life Cycle Initiative as a global body for the stewardship of impact assessment methods, delivering much-needed consensus-building among method developers and users at the interface between science and decision- and policy-making. It has been built with significant in-kind contribution of hundreds of experts in the last few years. More practically, it provides the necessary access to internationally endorsed, scientifically robust, and stable indicators so that life cycle assessment users can incorporate them in their studies.

UN Environment deeply appreciates the continued collaboration with the Society for Environmental Toxicology and Chemistry (SETAC), as well as from the whole life cycle community. This inclusive cooperation enhances the relevance and accuracy of life cycle approaches to informing the pathways towards sustainable consumption and production as mandated by the international community.

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Foreword - SETAC

As the world looks for ways to protect and manage the earth we live in, life cycle impact assessment (LCIA) has risen as a viable approach to utilize. LCIA provides a means to assess the impact of materials and processes on the well-being of humans and our environment. LCIA methodology ensures in-depth consideration of major impacts of products and technologies as well as integration of these impacts. This in turn enables users to understand broadly the health and environmental implications of these products and technologies. Therefore, LCIA enables decision makers, the public, and other stakeholders to make informed decisions based on better understanding the overall profile of a particular product or technology and its effect on the environment. The shared understanding that comes with a common vision is central to fostering informed dialogues and clear pathways toward decisions that involve the various parties who may benefit or be affected by a product or technology.

SETAC highly values our partnership with the Life Cycle Initiative at United Nations Environment to strengthen and advance LCIA. The SETAC Pellston Workshop conducted in the 2018 in Valencia Spain resulting in the Global Guidance on Environmental Life Cycle Impact Assessment Indicators – Volume 2 marks a great milestone in that collaboration. The impact areas covered in Volume 2 of the guidance embrace a broad range of stressors that impinge on the health and wellbeing of humans and their environment. The guidance defines approaches for assessing impacts regarding acidification and eutrophication, human toxicity, natural mineral resources, ecosystem services related to soils, ecotoxicity, and integration across these impact areas. Moreover, it includes much needed explicit consideration of variability and uncertainty in LCIA. The impact areas advanced in Volume 2 make a great complement to those defined in Volume 1 and can be directly linked to the UN Environment Sustainable Development Goals.

Keeping LCIA useful and fresh means simultaneously establishing and advancing impact approaches and also having a process for periodically updating approaches with emerging scientific knowledge. The Life Cycle Initiative operating within the partnership forged between UN Environment and SETAC provides a good foundation for this longer-term effort. SETAC is proud to help advance LCIA methods and applications. SETAC places emphasis on fostering research in environmental sciences as well as the application of the latest scientific advances for decision making and environmental management and advancing LCIA methods and application is an excellent fit to our mission. It will be interesting to explore how LCIA can be linked and leveraged to inform decisions to manage and protect our environment. SETAC looks forward to a continued working relationship with the Life Cycle Initiative to help promote and advance this important field of assessment.

Charlie Menzie
SETAC Executive Director

Abbreviations and Acronyms

ACF	Accessibility factor
ACR	Acute-to-chronic ratio
AGWP	Absolute global warming potential
AoP	Area of protection
AR	Assessment report
BF	Bioavailability factor
BLM	Biotic ligand model
BMD	Benchmark dose
BOD	Biological oxygen demand
CBD	Convention on Biological Diversity
CF	Characterisation factor
CI	Confidence interval
CMB	Conditions to maintain biodiversity
CMR	Carcinogenicity, mutagenicity, and reproductive/developmental toxicity
COD	Chemical oxygen demand
ConsExpo	Consumer Exposure assessment tool
CTUe	Comparative Toxic Unit for ecotoxicity
DALY	Disability-adjusted life year
DIN	Dissolved inorganic nitrogen
DIP	Dissolved inorganic phosphorus
DOC	Dissolved organic carbon
DON	Dissolved organic nitrogen
DOP	Dissolved organic phosphorus
DRF	Dose-response function
EC10	Effect concentration affecting 10% of individuals above background
EC10eq	EC10 equivalent; equivalent of chronic effect concentration affecting 10% of individuals above background
EC20	Effect concentration affecting 20% of individuals above background
EC50	Effect concentration affecting 50% of individuals above background
ECx	Effect concentration affecting x% of individuals above background
$ED10_H$	Effect dose inducing a 10% response over background in humans
$ED1_H$	Effect dose inducing a 1% response over background in humans
ED50	Effect dose inducing a 50% response over background
$ED50_H$	Effect dose inducing a 50% response over background in humans
EF	Effect factor
FAO	Food and Agriculture Organization of the United Nations
FF	Fate factor
FIAM	Free ion activity model
FU	Functional unit

GBD	Global burden of disease
HANPP	Human appropriation of net primary productivity
HC5	Hazardous concentration exposing 5% of species above given effect concentration
HC20	Hazardous concentration exposing 20% of species above given effect concentration
HC50	Hazardous concentration exposing 50% of species above given effect concentration
HTS	High-throughput screening
iF	Intake fraction
IPCC	Intergovernmental Panel on Climate Change
IPCS	International Programme on Chemical Safety
ISES	International Society of Exposure Science
ISO	International Organization for Standardisation
IUCN	International Union for Conservation of Nature
IVIVE	In vitro to in vivo extrapolation
LCA	Life cycle assessment
LCI	Life cycle inventory analysis
LCIA	Life cycle impact assessment
LEAP	Livestock Environmental Assessment and Performance Partnership
L(E)C50	Lethal effect concentration affecting 50% of the individuals above background
LME	Large marine ecosystems
LOEC	Lowest observed effect concentration
LU	Land use
LUC	Land use change
LULUC	Land use and land use change
MATC	Maximum acceptable toxicant concentration
MEA	Millennium Ecosystem Assessment
msPAF	Multisubstance potentially affected fraction (of species)
NAM	New approach methodologies
NCCT	National Center for Computational Toxicology
NOAEL	No observable adverse effect level
NOEC	No observed effect concentration
NPP	Net primary productivity
NTCF	Near-term climate forcer
PAF	Potentially affected fraction (of species)
PDF	Potentially disappeared fraction (of species)
PFAS	Polyfluoroalkyl substances
PiF	Product intake fraction
PM2.5	Fine particulate matter: Particles with aerodynamic diameter ≤2.5 µm
PNEC	Predicted no effect concentration
PNOF	Potentially non-occurring fraction (of species)

PNV	Potential natural vegetation
POD	Point of departure
QSAR	Quantitative structure-activity relationships
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RSR	Relative species richness
RUSLE	Revised universal soil loss equation
SAR	Species-area relationship
SETAC	Society for Environmental Toxicology and Chemistry
SF	Severity factor
SHEDS	Stochastic human exposure and dose simulation model
SOC	Soil organic carbon
SOM	Soil organic matter
SP	Suspended particles
SSD	Species sensitivity distribution
STP	Solid waste treatment plant
SVOC	Semi-volatile organic compound
TD50	Median tumour dose
TH	Time horizon
TTC	Threshold of toxicological concern
UN	United Nations
UNEP	United Nations Environment Programme (aka UN Environment)
US EPA	United States Environmental Protection Agency
USEtox	UNEP-SETAC scientific consensus model for human toxicity and ecotoxicity characterization
WHO	World Health Organisation
WMGHG	Well-mixed greenhouse gas
WWF	World Wide Fund for Nature
WWTP	Wastewater treatment

Executive summary

Background

Reducing the environmental impacts from consumption and production systems is a priority of the 2030 Agenda for Sustainable Development. This requires developing products and services with reduced impacts to human health and the environment. Accordingly, guidance is needed on which quantitative life cycle based indicators are best suited to measure and monitor impacts on human health, ecosystems and natural resources.

Approach

The Life Cycle Initiative, hosted by UN Environment, initiated a global process in 2013 to reach consensus on recommended environmental indicators and characterisation factors (CFs) for life cycle impact assessment (LCIA). Four initial topics (selected based on their perceived environmental or political relevance, the maturity of available quantitative indicators, and the likelihood of reaching consensus) were discussed in international task forces for 24 months before concluding with the publication of Global Guidance for Life Cycle Impact Assessment Indicators Volume 1 (Frischknecht & Jolliet 2017; Jolliet et al. 2018). The four topics were climate change, fine particulate matter impacts on human health, water use impacts (scarcity and human health impacts), and land use impacts on biodiversity. The same process was replicated for additional environmental topics between 2016-2018, namely 1) acidification and eutrophication, 2) human toxicity 3) mineral resources 4) soil quality and related ecosystem services, 5) ecotoxicity, as well as 6) crosscutting issues. The Pellston Workshop for these topics, held 24th-29th June 2018 in Valencia, Spain, included domain experts, LCIA method developers, consultants, industry associations, and users of life cycle information, including intergovernmental organisations (IGOs), government, industry, nongovernmental organisations (NGOs), and academics. Balance was maintained between scientific rigour and practicality, to bridge the gap between scientific complexity and the call for concise, meaningful and well-tested environmental indicators, while carefully defining the domain of applicability for which the developed indicators are appropriate.

Summary results

The participants of the Pellston Workshop agreed on the following main tangible recommendations for the environmental indicators, including substantial innovations.

Human toxicity: Three human toxicity indicators are recommended considering severity for cancer, reproductive/developmental, and other non-cancer effects. For human exposure, these indicators build on a matrix framework coupling environmentally mediated exposures with indoor and consumer product exposures. The non-cancer indicators build on a stochastic dose-response model recommended by the World Health Organization for a 10% population response level to derive effect factors, combined with severity factors based on the latest Global Burden of Disease statistics.

Ecotoxicity: The major recommendations are to 1) consider effects of chemicals on organisms living in coastal waters, soil, freshwater and freshwater sediment; 2) base effect modelling on most available chronic data and concentration levels close to environmental concentrations; 3) disregard concentration reduction through bioaccumulation in exposure modelling, and 4) consider ageing and weathering of metals in soil and freshwater sediment.

Acidification and Eutrophication: Selected indicators and CFs are recommended for freshwater eutrophication, terrestrial acidification, and midpoint marine eutrophication. Other consensus recommendations are to 1) use spatially explicit models with global coverage, 2) aggregate CFs (to country or global level) using agricultural, non-agricultural, or overall emissions weighting, and 3) use existing environmental concentrations for effect modelling.

Soil quality and related ecosystem services: Soil organic carbon is the interim recommendation for soil quality. By refining the evaluation of forestry and permanent crops in LCIA to allow for the representation of improved land management this indicator may move to full recommendation. Finally, soil loss is recommended as a separate indicator linked to natural resources, in order to address erosion impacts.

Mineral resources: Methods have been grouped depending on whether they assess the impacts of a product system's resource use on the opportunities of future generations to use resources (inside-out) or resource availability for a product system (outside-in). For the inside-out perspective, Abiotic Depletion Potential is recommended to assess the depletion of stocks; interim recommendations are provided for additional perspectives (declining resource quality; economic externalities; thermodynamics). Methods addressing the outside-in perspective are recommended to complement (environmental) LCA studies.

Crosscutting issues: For uncertainties, it is strongly recommended to follow a tiered approach, interpreting and reporting all relevant types of uncertainty and associated variability. For harmonisation, it is strongly recommended to develop a common reference nomenclature and classification system for life cycle inventory analysis (LCI) and LCIA. Further research is recommended on improving available options for the instrumental values framework and addressing ecosystem vulnerability consistently, to allow aggregation of indicator scores across impacts.

Outlook and roadmap

The recommended environmental indicators represent the current best available knowledge and practice. It is strongly recommended 1) that the Life Cycle Initiative fosters the momentum of co-operation and establishes a community of LCIA researchers and users who act as stewards for these indicators; and 2) to integrate the set of indicators developed into a fully consistent and comprehensive LCIA global method. The implementation of the indicators in LCA software and databases asks for quality assurance measures such as verification and standard nomenclatures. Spatially differentiated indicators (e.g., ecotoxicity and soil quality) call for parsimonious approaches from the knowledge gained in LCA research projects in which a high geographic resolution is applied to common LCA studies where geographic information is often lacking.

These indicators are highly relevant to the UN's Sustainable Development Goals, to quantify and monitor progress towards sustainable production and consumption: governments and non-state actors are called to invest in their continued development and maintenance.

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Résumé Exécutif

Contexte

Réduire les impacts environnementaux des systèmes de consommation et de production est l'une des priorités du Programme de développement durable à l'horizon 2030. Il s'agit, pour y parvenir, de mettre au point des produits et des services ayant de faibles incidences sur la santé humaine et l'environnement. Des lignes directrices sont donc nécessaires afin de déterminer quels indicateurs en lien avec le cycle de vie sont les mieux adaptés pour mesurer et suivre les impacts sur la santé humaine, les écosystèmes et les ressources naturelles.

Approche

En 2013, l'Initiative Cycle de Vie (*Life Cycle Initiative*), organisée par ONU-Environnement, a lancé à l'échelle mondiale un processus visant à parvenir à un consensus sur les indicateurs et facteurs de caractérisation environnementaux recommandés pour l'analyse d'impact de cycle de vie (AICV). Quatre premières thématiques (sélectionnées au regard de leur pertinence environnementale ou politique estimée, ainsi que de la maturité des indicateurs quantitatifs disponibles et de la probabilité de parvenir au consensus recherché) ont été débattues au sein d'équipes spéciales internationales pendant 24 mois, à l'issue desquels le document *Global Guidance for Life Cycle Impact Assessment Indicators Volume 1* (Frischknecht & Jolliet 2017 ; Jolliet et coll. 2018) a été publié. Ces thématiques étaient les suivantes : (1) changements climatiques, (2) impacts des particules fines sur la santé humaine, (3) impacts de l'utilisation des ressources en eau (appauvrissement des ressources en eau et effets sur la santé humaine), et (4) impacts de l'utilisation des terres sur la biodiversité. D'autres thématiques environnementales ont été soumises au même processus entre 2016 et 2018 : (1) acidification et eutrophisation ; (2) toxicité humaine ; (3) ressources minérales ; (4) qualité des sols et des services écosystémiques associés ; (5) écotoxicité ; et (6) autres questions transversales. L'atelier de consensus (ou *Pellston Workshop*) sur ces sujets, qui s'est tenu du 24 au 29 juin 2018 à Valence (Espagne), a rassemblé des experts des domaines concernés, des chargés du développement de la méthode AICV, des consultants, des associations du secteur industriel, ainsi que des utilisateurs des informations sur le cycle de vie – organisations intergouvernementales, gouvernements, industrie, organisations non gouvernementales (ONG), et universitaires. Un équilibre a été maintenu entre la rigueur scientifique et les aspects concrets, afin que la complexité scientifique puisse aller de pair avec la nécessité d'indicateurs environnementaux concis, significatifs et éprouvés ; en parallèle, le domaine d'applicabilité adapté a été soigneusement défini pour chaque indicateur.

Principaux résultats

Les participants du *Pellston Workshop* ont convenu de formuler à l'égard des indicateurs environnementaux les principales recommandations concrètes ci-après, qui comportent des innovations conséquentes.

Toxicité humaine : Trois indicateurs de toxicité humaine sont recommandés comprenant la gravité d'un cancer, les effets sur la reproduction/le développement, et les effets non cancérogènes. En ce qui concerne l'exposition humaine, ces indicateurs s'appuient sur un cadre matriciel associant les expositions environnementales, en extérieur et en intérieur, et l'exposition via des produits de consommation. Les indicateurs des effets non cancérogènes s'appuient quant à eux sur un modèle stochastique dose-réponse recommandé par l'Organisation Mondiale de la Santé (OMS) pour un taux de population sensible de 10 %, dont sont déduits des facteurs d'effets, auxquels sont associés des facteurs de gravité selon les dernières statistiques mondiales sur la charge de morbidité.

Ecotoxicité : les principales recommandations sont de (1) prendre en compte les effets des produits chimiques sur les organismes vivant dans les eaux côtières, le sol, les eaux douces et les sédiments d'eau douce, (2) fonder la modélisation des effets majoritairement sur les données disponibles sur l'écotoxicité chronique ainsi que sur des niveaux de concentration proches des concentrations environnementales, (3) ne pas tenir compte de la baisse de concentration par bioaccumulation dans la modélisation de l'exposition, et (4) tenir compte du vieillissement et de la dégradation des métaux dans le sol et les sédiments d'eau douce.

Acidification et eutrophisation : certains indicateurs et facteurs de caractérisation sont recommandés pour l'eutrophisation des eaux douces, l'acidification terrestre et l'eutrophisation marine intermédiaire. Il est en outre recommandé (1) d'utiliser des modèles spatialement explicites dont le champ d'application est mondial, (2) d'agréger les facteurs de caractérisation (au niveau national ou mondial) en appliquant une pondération des émissions agricoles, non agricoles ou totales, et (3) de s'appuyer sur les concentrations environnementales existantes pour la modélisation des effets.

Qualité des sols et des services écosystémiques associés : le carbone organique du sol est recommandé temporairement comme indicateur de la qualité du sol. Si, dans le cadre de l'AICV, l'évaluation de la foresterie et des cultures permanentes est affinée pour permettre la représentation de la gestion améliorée des terres, cet indicateur pourrait être pleinement recommandé. Enfin, la perte de sol est recommandée comme indicateur distinct pour les ressources naturelles, afin de mesurer les impacts en termes d'érosion.

Ressources minérales : plusieurs méthodes ont été regroupées, selon qu'elles évaluent les impacts de l'utilisation d'une ressource d'un système de produits sur les possibilités pour les futures générations d'utiliser les ressources (perspective de l'intérieur vers l'extérieur), ou la disponibilité d'une ressource pour un système de produits (perspective de l'extérieur vers l'intérieur). Pour la perspective de l'intérieur vers l'extérieur, le potentiel de déplétion abiotique est recommandé pour évaluer l'épuisement des stocks ; d'autres indicateurs sont temporairement recommandés afin de disposer de perspectives supplémentaires (baisse de la qualité des ressources, externalités économiques, thermodynamique). Il est recommandé de compléter les études d'ACV (environnementales) par des méthodes intégrant la perspective de l'extérieur vers l'intérieur.

Questions transversales : en ce qui concerne les incertitudes, il est fortement recommandé de suivre une approche à plusieurs niveaux, et d'interpréter et signaler tous les types d'incertitude pertinents ainsi que la variabilité associée. Aux fins de l'harmonisation, il est fortement recommandé de mettre au point une nomenclature de référence commune et un système de classification pour l'analyse de l'inventaire du cycle de vie et l'AICV. Il est recommandé d'approfondir les recherches en vue d'améliorer les différentes possibilités qui s'offrent dans le cadre de valeurs instrumentales, et de traiter systématiquement de la vulnérabilité des écosystèmes, afin de permettre l'agrégation des scores des indicateurs de manière transversale pour l'ensemble des impacts.

Perspectives et feuille de route

Les indicateurs environnementaux recommandés sont le fruit des meilleures connaissances et pratiques actuellement disponibles. Il est fortement recommandé (1) que l'Initiative Cycle de Vie favorise l'élan donné par la coopération et établisse une communauté de chercheurs et d'utilisateurs de l'AICV qui jouent un rôle de gestionnaires de ces indicateurs, et (2) d'intégrer l'ensemble des indicateurs mis au point au sein d'une méthode d'AICV globale, pleinement cohérente et complète. La mise en oeuvre des indicateurs dans le logiciel et les bases de données d'ACV exige des mesures d'assurance qualité (vérification, nomenclatures normalisées). Les indicateurs différenciés selon une composante spatiale (écotoxicité et qualité du sol, par exemple) demandent de faire preuve de discernement entre les connaissances acquises dans le cadre de projets de recherche ACV à forte résolution géographique, et les études ACV courantes où les données géographiques font souvent défaut. Tous ces indicateurs sont extrêmement pertinents, au regard des Objectifs de développement durable définis par les Nations Unies, s'agissant de quantifier et de suivre les progrès réalisés en matière de production et de consommation durables : les gouvernements et acteurs non étatiques sont appelés à investir en faveur de leur développement et de leur maintien dans la durée.

Références

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Resumen ejecutivo

Antecedentes

La reducción de los efectos que los sistemas de consumo y producción tienen sobre el medio ambiente es una prioridad de la Agenda 2030 para el Desarrollo Sostenible. Para ello es necesario crear productos y servicios que afecten menos a la salud humana y al medio ambiente. Por consiguiente, se requiere orientación para determinar qué indicadores cuantitativos basados en el ciclo de vida son los más adecuados para evaluar y supervisar los efectos en la salud humana, los ecosistemas y los recursos naturales.

Enfoque

La Iniciativa del Ciclo de Vida, auspiciada por ONU-Medio Ambiente, inició un proceso mundial en 2013 para llegar a un consenso sobre los indicadores ambientales y los factores de caracterización recomendados para la evaluación de impacto del ciclo de vida. Cuatro temas iniciales (seleccionados según su pertinencia aparente para el medio ambiente o las políticas, la madurez de los indicadores cuantitativos disponibles, y la probabilidad de llegar a un consenso) fueron debatidos en grupos de trabajo internacionales durante 24 meses, concluyendo con la publicación del primer volumen de *Global Guidance for Life Cycle Impact Assessment Indicators* (Guía mundial para los indicadores de la evaluación de impacto del ciclo de vida) (Frischknecht & Jolliet 2017; Jolliet et al. 2018). Los cuatro temas fueron el cambio climático, el efecto de las partículas finas en la salud humana, las repercusiones del uso del agua (escasez y consecuencias para la salud humana) y las repercusiones del uso de la tierra para la biodiversidad. El mismo proceso se repitió para otros temas ambientales entre 2016 y 2018, a saber, 1) acidificación y eutrofización, 2) toxicidad humana, 3) recursos minerales, 4) calidad del suelo y servicios ecosistémicos conexos, 5) ecotoxicidad, y 6) cuestiones transversales. El Taller Pellston sobre estos temas, celebrado del 24 al 29 de junio de 2018 en Valencia (España), contó con la participación de expertos en la materia, creadores de métodos de evaluación de impacto del ciclo de vida, consultores, asociaciones del sector industrial, y usuarios de información sobre el ciclo de vida, incluidas organizaciones intergubernamentales (OIG), gobiernos, la industria, organizaciones no gubernamentales (ONG) y académicos. Se mantuvo el equilibrio entre el rigor científico y la practicidad, a fin de salvar la brecha entre la complejidad científica y la necesidad de contar con indicadores ambientales concisos, comprensibles y bien probados, al tiempo que se definía cuidadosamente el ámbito de aplicabilidad para el que son adecuados estos indicadores.

Síntesis de los resultados

Los participantes del Taller Pellston aprobaron las siguientes recomendaciones principales para los indicadores ambientales, incluyendo innovaciones sustanciales.

Toxicidad humana: se recomiendan tres indicadores de toxicidad humana teniendo en cuenta la gravedad para los efectos cancerígenos, reproductivos y de desarrollo, y no cancerígenos de otro tipo. Para la exposición humana, estos indicadores se basan en una matriz que combina las exposiciones en las que interviene el medio ambiente con las exposiciones en el interior y a productos de consumo. Los indicadores no cancerígenos reposan en un modelo dosis-respuesta estocástico recomendado por la Organización Mundial de la Salud para un nivel de respuesta de la población del 10%, con el fin de obtener factores de efecto, combinados con factores de gravedad basados en las estadísticas de la carga mundial de morbilidad más recientes.

Ecotoxicidad: las principales recomendaciones son: 1) tener en cuenta los efectos de los productos químicos sobre los organismos que viven en las aguas costeras, el suelo, el agua dulce y los sedimentos de agua dulce; 2) basar los modelos de efectos en los datos de efectos crónicos disponibles y los niveles de concentración cercanos a las concentraciones ambientales; 3) no tomar en consideración la reducción de la concentración mediante la bioacumulación en los modelos basados en el grado de exposición; y 4) considerar el envejecimiento y la erosión de los metales en el suelo y los sedimentos de agua dulce.

Acidificación y eutrofización: se recomiendan indicadores y factores de caracterización seleccionados para la eutrofización de agua dulce, la acidificación terrestre y la eutrofización marina. Otras recomendaciones por consenso son: 1) emplear modelos espacialmente explícitos con cobertura mundial, 2) agregar factores de caracterización (en el plano nacional o mundial) usando ponderaciones de emisiones agrícolas, no agrícolas o globales, y 3) utilizar las concentraciones ambientales existentes para los modelos de efectos.

Calidad del suelo y servicios de los ecosistemas: se recomienda el carbono orgánico del suelo como indicador interino de la calidad del suelo. Se recomienda perfeccionar la representación del efecto de la silvicultura y los cultivos permanentes sobre el carbono del suelo para mejorar la representación del uso de tierras, con el fin de convertir este indicador en una recomendación definitiva. Por último, se recomienda la pérdida de suelo como indicador vinculado a los recursos naturales, con miras a abordar los efectos de la erosión.

Recursos minerales: se han agrupado los métodos en función de si evalúan las repercusiones del uso de los recursos de un sistema de productos en las oportunidades de las generaciones futuras de utilizar los recursos (de adentro hacia afuera) o la disponibilidad de recursos para un sistema de productos (de afuera hacia adentro). Para la perspectiva de adentro hacia afuera, se recomienda el potencial de agotamiento abiótico para evaluar el agotamiento de las existencias; y se proporcionan recomendaciones provisionales para perspectivas adicionales (disminución de la calidad de los recursos; externalidades económicas; y termodinámica). Se recomiendan métodos que aborden la perspectiva de afuera hacia adentro para complementar los estudios (ambientales) de análisis de ciclo de vida (ACV).

Cuestiones transversales: para las incertidumbres, se recomienda encarecidamente aplicar un enfoque escalonado, interpretando y compartiendo todos los tipos pertinentes de incertidumbre y la variabilidad conexa. A fin de velar por la armonización, se recomienda firmemente formular una nomenclatura de referencia y un sistema de clasificación comunes para el análisis del inventario del ciclo de vida y la evaluación de impacto del ciclo de vida. Se recomienda una investigación más a fondo para mejorar las opciones disponibles para el marco instrumental de valores y abordar la vulnerabilidad de los ecosistemas de manera coherente, y así permitir la agregación de las puntuaciones de los indicadores de los distintos efectos.

Perspectivas y hoja de ruta

Los indicadores ambientales recomendados reflejan los mejores conocimientos y prácticas disponibles en la actualidad. Se recomienda enfáticamente 1) que la Iniciativa del Ciclo de Vida fomente el impulso de la cooperación y establezca una comunidad de investigadores y usuarios de la evaluación de impacto del ciclo de vida, que actúen de administradores de estos indicadores; y 2) que se integre el conjunto de indicadores elaborados en un método global de la evaluación de impacto del ciclo de vida plenamente coherente y completo. La aplicación de los indicadores en programas informáticos y bases de datos de ACV requiere medidas de garantía de calidad tales como la verificación y nomenclaturas estándar. Los indicadores espacialmente diferenciados (por ejemplo, la ecotoxicidad y la calidad del suelo) requieren enfoques parsimoniosos a partir del conocimiento adquirido en los proyectos de investigación de ACV en los que se aplica una alta resolución geográfica a estudios comunes de ACV en los que a menudo falta información geográfica.

Estos indicadores son muy pertinentes para los Objetivos de Desarrollo Sostenible de las Naciones Unidas, ya que permiten cuantificar y seguir el progreso hacia el logro de la producción y el consumo sostenibles. Por ello se exhorta a los gobiernos y los agentes no estatales a invertir en su perfeccionamiento y mantenimiento continuos.

Referencias

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Рабочее резюме

История вопроса

Снижение воздействия систем производства и потребления на окружающую среду является од-ним из приоритетов Повестки дня в области устойчивого развития на период до 2030 года. Это предполагает переход к производству товаров и оказанию услуг, в меньшей степени воздейству-ющих на здоровье человека и состояние окружающей среды. В связи с этим необходима мето-дология, которая позволила бы определить, какие количественные показатели, разработанные с учетом «жизненного цикла» продукции, лучше всего подходят для оценки и конт-роля оказываемо-го ее производством воздействия на здоровье человека, состояние экосистем и запасы природ-ных ресурсов.

Подход к решению проблемы

Реализуемая под эгидой Программы ООН по окружающей среде «Инициатива по применению концепции жизненного цикла» положила в 2013 году начало глобальным усилиям по достижению консенсуса в отношении «рекомендуемых экологических показателей» (РЭП) и «характеризую-щих факторов» (ХФ), используемых для оценки воздействия на протяжении жизненного цикла (ОВЖЦ). В течение двух лет международные целевые группы специалистов вели дискуссии пер-воначально по четырем темам (занимались отбором с учетом предполагаемого экологического воздействия или политической значимости, оценкой степени проработанности имеющихся коли-чественных показателей и анализом вероятности достижения консенсуса), завершившиеся пуб-ликацией первого тома «Общих рекомендаций по разработке показателей оценки воздействия на протяжении жизненного цикла» (Frischknecht & Jolliet 2017; Jolliet et al. 2018). Этими четырьмя темами были: последствия изменения климата, воздействие тонкодисперсных частиц на здоро-вье человека, водопользование и его последствия (дефицит водных ресурсов и его влияние на здоровье человека), землепользование и его последствия для биоразнообразия. Аналогичная работа велась в 2016-2018 гг. в отношении ряда других проблемных с экологической точки зре-ния тем, а именно: (1) закисление и эвтрофикация; (2) токсичность для организма человека; (3) использование минеральных ресурсов; (4) качество почв и связанных с этим экосистемных услуг; (5) экологическая токсичность; (6) вопросы междисциплинарного характера. В организован-ном 24-29 июня 2018 года в Валенсии, Испания, рабочем совещании приняли участие профиль-ные специалисты, разработчики метода ОВЖЦ, консультанты, отраслевые ассоциации, а также пользователи информации, касающейся оценки воздействия на протяжении жизненного цикла, включая представителей межправительственных организаций (МПО), правительственных струк-тур, частного сектора, неправительственных организаций (НПО) и академических кругов. При этом был соблюден баланс между строгим научным подходом к разработке показателей и их практической применимостью, что позволило решить сложную с научной точки зрения задачу и одновременно учесть просьбу, касавшуюся разработки «емких, эффективных и апробированных на практике экологических показателей с четким определением сферы их возможного примене-ния».

Резюме результатов совещания

Участники совещания согласовали следующие основные практические рекомендации в отноше-нии экологических показателей, в том числе важные инновационные подходы.

Токсичность для организма человека: Было рекомендовано использовать три показателя сте-пени токсичности для человека с учетом тяжести возможных последствий (онкологические забо-левания, репродуктивная токсичность/влияние на развитие организма, другие неонкологические последствия). Что касается воздействия на здоровье человека, то указанные показатели были оформлены в виде структурной матрицы, объединившей в себе факторы воздействия, оказывае-мого через окружающую среду, в закрытых помещениях и через потребительские товары. Пока-затели неонкологического воздействия были разработаны с использованием стохастической мо-дели зависимости «доза-реакция», рекомендованной Всемирной организацией здравоохранения в отношении 10-процентного показателя реагирования населения для определения воздейству-ющих факторов, а также факторов тяжести последствий, определяемых на основе последних статистических данных о глобальном бремени болезней.

Экологическая токсичность: Основные рекомендации: (1) принимать во внимание воздействие химических веществ на организмы, живущие в прибрежных водах, почве, пресной воде и пресно-водных отложениях; (2) модели предполагаемого воздействия рассчитывать на основе массива имеющихся данных о хроническом воздействии и уровнях концентрации, близких к предполагае-мой концентрации в окружающей среде; (3) при моделировании воздействия не учитывать сни-жение концентрации вследствие бионакопления; (4) принимать во внимание процесс старения и выветривания металлов в почве и пресноводных осадках.

Закисление и эвтрофикация: Для оценки эвтрофикации пресноводных водоемов, закисления почв и определения медианного значения эвтрофикации морской среды было рекомендовано использовать отдельные показатели и характеризующие факторы. В числе других, принятых на основе консенсуса рекомендаций, были следующие: (1) использовать пространственно выверен-ные модели с глобальным охватом, (2) группировать характеризующие факторы (на страновом или глобальном уровне) с использованием весового коэффициента для сельскохозяйственных, несельскохозяйственных или совокупных выбросов; (3) при моделировании воздействия использо-вать текущие показатели концентрации в окружающей среде.

Качество почв и связанных с этим экосистемных услуг: В качестве временного показателя состояния почв был рекомендован уровень содержания почвенного органического углерода. Усо-вершенствование методов оценки лесных ресурсов и постоянных культур в рамках ОВЖЦ в целях представления систем рационального землепользования, возможно, позволит закрепить за этим показателем статус полноценной рекомендации. Наконец, в интересах борьбы с последствиями эрозии почв показатель потери почвы был рекомендован в качестве отдельного, связанного с природными ресурсами показателя.

Использование минеральных ресурсов: Методы были сгруппированы с учетом того, оценива-ются ли с их помощью последствия использования минеральных ресурсов в системе производ-ства с точки зрения перспективы их использования будущими поколениями (принцип «ориентации на потребности») или же с точки зрения наличия таких ресурсов для использования в системе производства (принцип «ориентации на возможности»). Что касается принципа «ориентации на потребности», то для оценки истощенности запасов было рекомендовано использовать показа-тель потенциала абиотического истощения; в отношении других критериев оценки (снижение качества ресурсов, внешние экономические факторы, термодинамические аспекты) были предло-жены временные рекомендации. Методы оценки на основе принципа ориентации на возможно-сти было рекомендовано использовать при исследовании (экологических аспектов) ОЖЦ.

Вопросы междисциплинарного характера: В отношении учета факторов неопределенности было настоятельно рекомендовано применять многоуровневый подход, основанный на анализе и представлении данных относительно всех соответствующих категорий неопределенности и свя-занных с ними переменных факторов. В целях унификации было также настоятельно рекомендо-вано разработать общий понятийно-терминологический аппарат и систему классификации для обеспечения возможности инвентаризационного анализа жизненного цикла (ИАЖЦ) и оценки воздействия на протяжении жизненного цикла (ОВЖЦ). Кроме того, было рекомендовано про-должить изучение возможностей совершенствования существующей системы инструментальных ценностей и последовательного решения проблемы уязвимости экосистем, что позволит агреги-ровать значения показателей по всем типам воздействия.

Перспективы и общие направления работы

Рекомендуемые экологические показатели разработаны на основе наиболее эффективных на сегодняшний день методов и практических подходов. Настоятельно рекомендуется (1) содействовать тому, чтобы Инициатива по применению концепции жизненного цикла стиму-лировала развитие сотрудничества и формирование сообщества исследователей и пользовате-лей показателей ОВЖЦ, выступающих в качестве кураторов их внедрения; (2) интегрировать набор разработанных показателей в полностью согласованную на глобальном уровне всеобъем-лющую методологию ОВЖЦ. Внедрение показателей в информационные системы и базы дан-ных ОЖЦ потребует принятия мер по обеспечению качества, в частности, выверки данных и ис-пользования стандартной терминологии. Подготовка пространственно дифференцированных показателей (таких как «экологическая токсичность» и «качество почвы») требует применения эко-номичных подходов, основанных на использовании данных, полученных в рамках исследователь-ских проектов в области ОЖЦ, в которых высокое географическое разрешение применяется для проведения общих исследований по ОЖЦ, нередко сталкивающихся с проблемой недостатка географических данных. Представленные показатели имеют самое непосредственное отноше-ние к достижению утвержденных ООН целей в области устойчивого развития и необходимы для проведения количественной оценки и обеспечения мониторинга прогресса в процессе перехода к устойчивым моделям производства и потребления. Правительствам и негосударственным струк-турам предлагается оказать поддержку, необходимую для их постоянного совершенствования и актуализации.

Использованная литература

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执行摘要

背 景

降低消费和生产系统对环境的影响，是《2030年可持续发展议程》的一个优先事项。做好这项工作，需要开发出对人类健康和环境影响较小的产品和服务。因此，有必要制定一份指南，以便确定哪些基于生命周期的定量指标最适于衡量和监测对人类健康、生态系统和自然资源的影响。

方法

由联合国环境署主持的“生命周期倡议”计划于2013年开启了一个全球进程，旨在针对为开展生命周期影响评估所推荐的环境指标和特征化因素达成共识。国际工作组对（根据预估的环境或政治相关性、现有定量指标的成熟度和达成共识的可能性选取的）四个初始议题进行了长达24个月的讨论，最终出版了《生命周期影响评估指标全球指南》第1卷（Frischknecht&Jolliet 2017; Jolliet et al. 2018）。这四个议题是：气候变化、细颗粒物对人类健康的影响、水使用所产生的影响（水源稀缺性及其对人类健康的影响）、土地利用对生物多样性的影响。2016-2018年，该工作组对其他环境议题采取了同样程序，这些议题是：1）酸化和富营养化；2）人体毒性；3）矿产资源；4）土壤质量和相关的生态系统服务；5）生态毒性；6）跨领域问题。2018年6月24-29日，在西班牙瓦伦西亚举行了有关上述议题的佩尔斯顿研讨会TM，与会者包括相关领域专家、生命周期影响评估方法开发人员、顾问、行业协会，以及政府间组织、政府、行业、非政府组织和学者等生命周期信息用户。为弥合科学复杂性与需要，制定简明、有意义和经过充分检验的环境指标之间的差距，妥善兼顾了科学严谨性与实用性，同时审慎界定了指标的适用范围。

成果综述

佩尔斯顿研讨会TM的与会者同意针对环境指标提出以下几项主要建议，其中包括一些实质性创新。

人体毒性：考虑到生殖/发育性癌症的严重性及其他非癌症影响，推荐三个人体毒性指标。就人体接触而言，这些指标建立在结合了环境介导接触与室内接触和消费品接触的综合框架之上。非癌症指标则建立在世界卫生组织推荐的随机剂量反应模型之上，该模型以10%的人口回应率得出影响因素，同时结合了基于全球疾病负担最新统计数据的疾病严重程度因素。

生态毒性：主要建议是：1）考虑化学品对生活在近海水域、土壤、淡水和淡水沉积物中的生物的影响；2）效应建模以现有的大部分长期数据和接近环境浓度的浓度水平为基础；3）在接触建模中忽略由于生物积累而发生的浓度降低；4）考虑土壤和淡水沉积物中金属的老化和风化。

酸化和富营养化：为淡水富营养化、陆地酸化和中点海洋富营养化推荐选定的指标和特征化因素。其他协商一致的建议包括：1）使用覆盖全球的空间直观模型；2）利用农业、非农业或总体排放权重对特征化因素进行（国家或全球一级）总计；3）使用现有环境浓度进行效应建模。

土壤质量和相关的生态系统服务：暂时建议将土壤有机碳作为土壤质量指标。如果在生命周期影响评估中通过完善林业和永久性作物评价可以体现改善后的土地管理情况，这一指标即可成为正式推荐的指标。最后，建议将土壤流失作为与自然资源有关的单独指标，以便表示侵蚀的影响。

矿产资源：根据评估内容不同采用不同方法，如果是评估产品系统的资源利用对后代利用资源机会的影响，采用由内向外的方法；如果是评估资源可用性对产品系统的影响，则采用由外向内的方法。采用由内向外方法的时候，建议用非生物耗竭潜势来评估资源耗竭。还提出了临时建议，作为补充性方法（资源质量下降、经济外部性、热力学）。建议采用由外向内的方法，对（环境）生命周期评估研究加以补充。

跨领域问题：对于不确定性，强烈建议采用多层次办法，解释并报告所有相关类型的不确定性和相关的可变性。为了协调一致，强烈建议为生命周期清单（LCI）分析和生命周期影响评估开发一个通用的参考命名和分类系统。建议进一步研究如何改进现有的工具性价值框架选项并始终如一地应对生态系统脆弱性问题，从而能够将各种影响的指标得分进行合计。

展望与路线图

本报告所推荐的环境指标代表着现有的最佳知识和实践。强烈建议：1）“生命周期倡议”计划促进合作机遇，并建立一个生命周期影响评估研究人员和用户群体，由他们作为这些指标的管理员；2）将所制定的这组指标综合起来，形成一个统一且全面的生命周期影响评估全球方法。将这些指标应用于生命周期评估软件和数据库，需要采用验证和标准命名法等质量保证措施。空间差异指标（例如生态毒性和土壤质量）需要根据从生命周期评估研究项目中获得的知识总结出的简约方法。在这些项目里，高地理解析度被应用于通常缺乏地理信息的常规生命周期评估研究当中。

这些指标与联合国可持续发展目标高度相关，旨在量化并监测实现可持续生产和消费的进展：我们呼吁各国政府和非政府机构不断开发和维护这些指标。

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Executive summary (Arabic)

نوعية التربة وخدمات النظام الإيكولوجي المرتبطة بها: يوصى باستخدام الكربون العضوي في التربة كمؤشر مؤقت لنوعية التربة. ومن خلال تحسين تقييم الغابات والمحاصيل الدائمة في مؤشرات تقييم الآثار من منظور دورة الحياة لإتاحة تمثيل إدارة الأراضي المحسَّنة، قد يرتقي هذا المؤشر إلى مستوى التوصية الكاملة. وأخيراً، يوصى باستخدام فقدان التربة كمؤشر منفصل مرتبط

بالموارد الطبيعية، من أجل معالجة آثار التآكل.

الموارد المعدنية: جرى تجميع الطرق المستخدمة في فئات بناء على ما إذا كانت تقيّم آثار استخدام موارد نظام للمنتجات على فرص استخدام الأجيال المقبلة للموارد (اتجاه الداخل إلى الخارج) أو على مدى توفر الموارد لنظام المنتجات (اتجاه الخارج إلى الداخل). فبالنسبة لمنظور الداخل إلى الخارج، يوصى باستخدام استنفاد الإمكانيات اللاأحيائية لتقييم نضوب المخزونات؛ ووضعت توصيات مؤقتة لوجهات نظر إضافية (تدهور جودة الموارد، العوامل الخارجية الاقتصادية، الديناميكا الحرارية). أما الطرق التي تتناول منظور الخارج إلى الداخل فيوصى باستخدامها لاستكمال دراسات تقييم دورة الحياة (البيئية).

المسائل الشاملة: فيما يتعلق بحالات عدم اليقين، يوصى بشدة باتباع نهوج متعدد المستويات، وتفسير جميع أنواع عدم اليقين ذات الصلة والتغير المرتبط بها والإبلاغ عنها. ولأغراض المواءمة، يوصى بشدة بوضع نظام مرجعي موحَّد للتسميات والتصنيف لتحليل قائمة دورة الحياة وتقييم الآثار من منظور دورة الحياة. ويوصى بإجراء مزيد من البحوث فيما يتعلق بتحسين الخيارات المتاحة لإطار القيم الفعالة والمعالجة المنتظمة لهشاشة النظام الإيكولوجي، من أجل السماح بتجميع درجات المؤشرات لكافة التأثيرات.

التوقعات وخريطة الطريق

تمثل المؤشرات البيئية الموصى بها أفضل المعارف والممارسات المتاحة في الوقت الحالي. ويوصى بشدة بما يلي: (١) أن تعزز مبادرة دورة الحياة زخم التعاون وتوجِد مجتمعاً من الباحثين والمستخدمين في مجال تقييم الآثار من منظور دورة الحياة يكونون بمثابة مسؤولين عن هذه المؤشرات؛ (٢) دمج مجموعة المؤشرات التي تم وضعها في طريقة عالمية شاملة ومتسقة تماماً للتقييم الآثار من منظور دورة الحياة. ويقتضي تطبيق المؤشرات في برامج تقييم دورة الحياة وقواعد البيانات الخاصة به تدابير ضمان الجودة من قبيل التحقق والتسميات الموحَّدة. وتقتضي المؤشرات التي تختلف حسب الأماكن (مثل السمية الإيكولوجية ونوعية التربة) اتباع نُهوج دقيقة من المعارف المكتسبة في مشاريع بحوث تقييم دورة الحياة تطبَّق فيها درجة عالية من الدقة الجغرافية على الدراسات الشائعة في مجال تقييم دورة الحياة التي كثيراً ما تنقصها المعلومات الجغرافية.

ولهذه المؤشرات أهمية كبيرة بالنسبة لأهداف الأمم المتحدة للتنمية المستدامة، من أجل قياس ورصد التقدم المحرز نحو الإنتاج والاستهلاك المستدامين: والحكومات والجهات الفاعلة غير الحكومية مدعوة إلى الاستثمار في مواصلة تطويرها والعناية بها.

المراجع

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موجز تنفيذي

خلفيـة

يمثل الحد من الآثار البيئية الناجمة عن أنظمة الاستهلاك والإنتاج إحدى الأولويات في خطة التنمية المستدامة لعام ٢٠٣٠. ويتطلب ذلك إيجاد منتجات وخدمات منخفضة التأثير على صحة الإنسان وعلى البيئة. ومن ثم، هناك حاجة إلى توجيه فيما يتعلق بأكثر المؤشرات الكمية المستندة إلى دورة الحياة ملاءمةً لقياس ورصد الآثار على صحة الإنسان والنظم الإيكولوجية والموارد الطبيعية.

النهج المتَّبَع

بدأت مبادرة دورة الحياة، التي يستضيفها برنامج الأمم المتحدة للبيئة، عملية عالمية في عام ٢٠١٣ للتوصل إلى توافق في الآراء بشأن ما يوصى به من المؤشرات البيئية وعوامل التصنيف التي تستخدم لتقييم الآثار من منظور دورة الحياة. ونوقشت أربعة موضوعات أولية (تم اختيارها بناءً على تصوُّر أهميتها البيئية أو السياسية، ومدى نضج المؤشرات الكمية المتاحة، واحتمال التوصل إلى توافق في الآراء) في نطاق أفرقة عمل دولية لمدة ٢٤ شهراً قبل الانتهاء إلى إصدار المجلد ١ من المؤلَّف المعنون "توجيه عالمي بشأن مؤشرات تقييم الآثار من منظور دورة الحياة" (Frischknecht & Jolliet ؛٢٠١٧ Jolliet et al. ٢٠١٨). وتمثلت الموضوعات الأربعة المختارة في تغير المناخ، وآثار الجسيمات الدقيقة على صحة الإنسان، وآثار استخدام المياه (الندرة والآثار على صحة الإنسان)، وآثار استخدام الأراضي على التنوع البيولوجي. وتكرَّر إجراء نفس العملية في الفترة بين ٢٠١٦-٢٠١٨ بالنسبة للمواضيع البيئية الإضافية التالية: (١) التحمُّض والإتخام بالمغذيات، و(٢) السُمّيَّة بالنسبة للبشر، و(٣) الموارد المعدنية، و(٤) نوعية التربة وخدمات النظام الإيكولوجي المرتبطة بها، و(٥) السمية الإيكولوجية، و(٦) المسائل الشاملة. وقد شارك في حلقة عمل بيلستون TM التي عُقدت في فالنسيا لدراسة هذه الموضوعات، في الفترة من ٢٤ إلى ٢٩ يونيو/ حزيران ٢٠١٨، إسبانيا، بعض الخبراء في هذه الميادين، وواضعي طريقة مؤشرات تقييم الآثار من منظور دورة الحياة، والخبراء الاستشاريين، والرابطات الصناعية، ومستخدمي المعلومات المتعلقة بدورة الحياة، بما في ذلك المنظمات الحكومية الدولية، والحكومة، والصناعة، والمنظمات غير الحكومية، والأكاديميون. وحرص المشاركون على تحقيق توازن بين الصرامة العلمية والتطبيق العملي، توخياً لسد الفجوة بين التعقيد العلمي والحاجة إلى إيجاد مؤشرات بيئية موجزة ومفيدة ومختبرة جيداً، مع التزام الدقة في تحديد مجال التطبيق الذي تلائمه المؤشرات الموضوعة.

موجـز النتائج

اتفق المشاركون في حلقة عمل بيلستون TM على التوصيات الملموسة الرئيسية التالية بشأن المؤشرات البيئية، وهي تشمل بعض تجديدات جوهرية.

السُمّية بالنسبة للبشر: يوصى باستخدام ثلاثة مؤشرات للسمية بالنسبة للبشر تتعلق بدراسة مدى شدة الآثار السرطانية والآثار الإنجابية/النمائية، والآثار غير السرطانية الأخرى. وفيما يتعلق بالتعرض البشري، تعتمد هذه المؤشرات على إطار مصفوفة للربط بين حالات التعرض عن طريق البيئة وحالات التعرض داخل المباني والتعرض للمنتجات الاستهلاكية. وتعتمد المؤشرات غير المتعلقة بالسرطان على الجمع بين نموذج عشوائية الاستجابة للجرعات الذي أوصت به منظمة الصحة العالمية، باستخدام مستوى استجابة نسبته ١٠٪ من مجموعة التجربة لاشتقاق عوامل التأثير، وبين عوامل شدة الإصابة استناداً إلى أحدث إحصاءات العبء العالمي للمرض.

السمية الإيكولوجية: تتمثل التوصيات الرئيسية فيما يلي: (١) دراسة آثار المواد الكيميائية على الكائنات الحية التي تعيش في المياه الساحلية والتربة والمياه العذبة ورواسب المياه العذبة؛ (٢) وضع نماذج التأثير بناء على أكثر البيانات المزمنة توافراً ومستويات التركيز القريبة من التركيزات البيئية؛ (٣) تجاهل خفض التركيز من خلال التراكم الأحيائي في وضع نماذج التعرض، (٤) إدخال القِدم الزمني وتعرض المعادن لعوامل التعرية في التربة ورواسب المياه العذبة في الاعتبار.

التحمُّض والإتخام بالمغذيات: يوصى باستخدام بعض المؤشرات والعوامل الوصفية بالنسبة للإتخام بالمغذيات في المياه العذبة، والتحمض البري، ونقطة المنتصف للإتخام البحري بالمغذيات. ومن التوصيات الأخرى التي حظيت بتوافق الآراء: (١) استخدام نماذج ذات تغطية عالمية تحدد بوضوح توزيع السمات الطبيعية، (٢) تجميع العوامل الوصفية (إلى المستوى القطري أو العالمي) باستخدام ترجيح الانبعاثات الزراعية، أو غير الزراعية، أو الإجمالية، (٣) استخدام التركيزات البيئية الحالية لوضع نماذج التأثير.

1. Context and Overview

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1.1 Scene set and objectives

The United Nations' General Assembly on Sustainable Development Goals (United Nations 2015) has set objectives for environmental stewardship at the global level, aiming at curbing unsustainable consumption and production patterns and ultimately transitioning to more sustainable lifestyles and livelihoods that benefit all. Many of these Sustainable Development Goals (SDGs) call for indicators to assess the present state and progress towards these goals.

With markets and supply chains increasingly globalised, clear and harmonised guidelines are needed at global level to ensure that the environmental impacts of products and services are quantified consistently. In particular, guidance is needed for the selection of the best-suited life cycle-based environmental indicators to quantify and monitor the impacts on climate change, biodiversity, water and mineral resources, acidification and eutrophication, toxicity, etc. The ongoing developments in the application of Life Cycle Assessment (LCA) methods to Product Environmental Footprint and to a wide range of products, calls for not only providing recommendations to method developers, but also to recommend a set of indicators that can then be used in such footprints within comprehensive Life Cycle Impact Assessment (LCIA) approaches. These indicators are expected to be used in environmental product information schemes, benchmarking in industry sectors, reporting by companies, intergovernmental and national environmental policies, and common LCA work commissioned by various stakeholders.

As stated in Jolliet et al. (2004), "Life Cycle Impact Assessment (LCIA) methods aim to connect, to the extent possible, emissions and extractions quantified in life cycle inventories (LCI-results) on the basis of impact pathways to their potential environmental damages. Impact pathways consist of linked environmental processes, and they express the causal chain of subsequent effects originating from an emission or extraction. According to ISO (International Organization for Standardization [ISO] 2006), LCI results are first classified into impact categories. A category indicator, representing the amount of impact potential, can be located at any place between the LCI results and the category endpoint."

To answer these needs, the Life Cycle Initiative hosted by UN Environment has been running the project Global Guidance on Environmental Life Cycle Impact Indicators, GLAM, to provide global guidance and build consensus on environmental Life Cycle Impact Assessment indicators. Initial project workshops in Yokohama 2012 and in Glasgow 2013, as well as a stakeholder consultation scoped the GLAM project (Jolliet et al. 2014). The first Global Guidance for Life Cycle Impact Assessment Indicators was issued in 2016. It proposed an updated LCIA framework (Verones et al. 2017) as well as indicators for climate change, water use impacts, health impacts of fine particulate, and impact of land use. The efforts resulted in the first set of consensus indicators covering the topics mentioned. The findings are documented in a Pellston report, a summarising scientific paper (Frischknecht and Jolliet 2016; Jolliet et al. 2018), as well as numerous publications on the topical indicators.

Some of these indicators have already been adopted by external stakeholders. For instance, the European Commission has incorporated the recommended water scarcity indicator "AWARE" and the indicator on human health impacts of fine particles. Additionally, Switzerland is using AWARE and the recommended biodiversity indicator for land use impacts to monitor the evolution of the country's environmental footprint (Frischknecht et al. 2018). This approach helps the government measure the success of its programs towards a more sustainable and green economy.

1.2 Objectives and working process

While the set of indicators from the first phase of this work helped address important environmental impacts, there is still a need to expand the set of covered indicators to other policy-relevant impact categories. To this end, the second phase of the consensus-finding process was launched soon after the first workshop in 2016. It started with a scoping phase and broad stakeholder consultations to identify the next priority areas.

This second cycle of global guidance aims to address the following areas, as identified during the consultations: a) human toxicity, b) ecotoxicity, c) acidification and eutrophication, d) soil quality and its impact on ecosystem services, e) mineral resources, and f) cross-cutting issues.

For each of these impact categories, and similar to the previous methodology, the main objective is to:

1. identify the scope of the work;
2. describe the impact pathway and review the existing indicators;
3. select the best-suited indicator or set of indicators based on well-defined criteria, and develop the method to quantify them on sound scientific basis;
4. provide characterisation factors with corresponding uncertainty and variability ranges;
5. apply the indicators to a common LCA case study to illustrate its domain of applicability;
6. provide recommendations in terms of indicators, status, and maturity of the recommended factors, applicability, link to inventory databases, roadmap for additional tests, and potential next steps.

To achieve these goals, more than 120 world-leading environmental and LCA scientists contributed to the activity. They were organized in five impact category-specific task forces (TFs) and complemented by a crosscutting issues TF. Multiple topical workshops and conferences were held by each individual TF to first scope the work and then develop scientifically robust indicators. These efforts were followed by three overarching workshops and stakeholder meetings in Nantes 2016, Brussels 2017 and Rome 2018, which were held in conjunction with the annual SETAC Europe annual meeting. They sought to address specific critical cross-cutting issues and collect stakeholder feedback from industry, administration, and academia.

The LCA case study on the production and consumption of rice (Frischknecht et al. 2016) developed during the first phase of consensus-finding is also used in this second phase. This LCA helps test the new impact category indicators identified by each TF and assess their practicality. The mineral resources Task Force made use of another more relevant case study, namely, driving an electric car (Stolz et al. 2016). This allowed them to assess a larger and more diverse set of minerals and metals.

This second phase of the consensus-finding process culminated in a one-week Pellston Workshop[1] in Valencia, Spain, 24–29 June 2018, where 39 experts and stakeholders from around the globe agreed on the recommended environmental indicators for each impact category described in this report.

1 See the Foreword by SETAC for additional description of the history and structure of SETAC Pellston Workshops.

1.3 Guiding principles for LCIA indicator harmonisation

There are numerous indicators that address environmental topics. As a first step, the following list of key features was used to identify environmental life cycle impact assessment indicators that qualify for being recommended:

- The indicators are aligned with an emitter, producer, or consumer perspective, because the environmental impacts are quantified relative to a functional unit (whether it is 1 pkm driven with an electric car in Switzerland or the preparation 1 kg of cooked rice).
- Environmental impacts depend on substance emissions obtained from the Life Cycle Inventory (LCI) analysis phase of LCA. The LCI analysis provides the mass aggregated emissions attributed to the functional unit of a product system across its supply chains and across its whole life cycle (manufacture, use, and end of life). Apart from a specification of the primary emission compartment (e.g., air, freshwater, seawater, groundwater, soil), there is limited geographical and temporal specification for most of the quantified emission and resource flows. This makes it difficult to characterise environmental impacts using non-linear dose-response functions.
- The purpose of LCA is to express the potential environmental impacts and damages associated with a product or service system in a way that supports comparisons between alternatives, both at the level of the individual substance emission and at the level of the entire studied system. In order to avoid introducing bias in LCA comparisons, LCIA focuses on representative or typical conditions, avoiding worst-case assumptions used to assure safety in activities such as pre-market regulatory assessments of chemicals.
- The aggregation of the environmental impact scores across the full life cycle and across substances emitted, or resources extracted or used, requires LCIA indicators and characterisation scores that are additive.

In the harmonisation process, the same global guiding principles, as those in the first guidance, were then applied on the identified LCIA indicators:

- *Environmental relevance* ensures that the scope covered by the recommended indicator addresses environmentally important issues.

- *Completeness* ensures that the recommended indicator covers a maximum achievable part of the corresponding environmental issue and has a global coverage.
- *Scientific robustness, evidence, validity, and certainty* ensure that the recommended indicator follows current knowledge and evidence rather than opinions, subjective or arbitrary choices, or normative assumptions.
- *Documentation, transparency, and reproducibility* ensure that the scientific principles, models, and data supporting the recommended indicator are accessible to third parties and thus facilitate review and quality assurance.
- *Applicability* ensures that the recommended approach can easily be implemented in LCA software, LCA databases, and corporate environmental management systems and supports the environmental assessment of complex supply chains including a large variety of background processes.
- *Level of experience* ensures that the recommended indicator has been applied in a number of sufficiently diverse LCA case studies and thus has proven its practicality.
- *Stakeholder acceptance* ensures that the recommended indicator is applied in LCA-related work carried out or commissioned by industry, administration, and non-governmental organisations, and in communication to businesses and consumers.

The present report does not provide a complete set of environmental life cycle impact assessment indicators; it covers only the five indicators mentioned above. The fact that this report includes guidance on indicators covering the five topical areas human toxicity, ecotoxicity, acidification and eutrophication, soil quality and its impact on ecosystem services, and mineral resources is not to be interpreted as an implicit expression of preference on these topics over others such as noise or nutritional impacts. It is neither an implicit encouragement to use only one or a limited sub-set of the recommended environmental impact category indicators.

When performing a product or organisational LCA it is highly recommended to use a broad set of environmental impact category indicators. This set should be tailored to its goal and scope and suited to address the variety of material environmental impacts that are expected from the activities of the organisation and the supply chain of the product, respectively.

1.4 Link to life cycle inventory analysis

In the past, LCI and LCIA were often developed independently. On the other hand, environmental impact category indicators are increasingly expected to include higher granularity, which requires extensive data collection efforts.

This is why special attention was given to the link between the recommended environmental impact category indicators and the current capabilities and constraints of existing LCI databases. First, a large number among the participants in the GLAM project have long-term LCI database experiences. Second, the use of the rice LCA case study ensured a consistent linkage between LCI and LCIA. This case study also helped test the indicators applicability, in particular:

- Traditional rice cultivation requires pesticides, hence provided an excellent basis for testing candidate and recommended indicators proposed by the human toxicity and ecotoxicity Task Forces.
- Rice cultivation requires fertilisation and causes nitrogen and phosphorous emissions, therefore helped the acidification and eutrophication Task Force to test their candidate and recommended indicators.
- Rice cultivation may affect the soil quality and thus provided a good basis to test approaches quantifying impacts on ecosystem services.
- The supply chain is sufficiently complex to urge the experts to provide regionalised factors as well as default factors, applicable to situations with limited or no geographic or temporal information.

The rice supply chain does not require a large range of mineral resources. Therefore, the Task Force on mineral resources relied on a different case study – driving an electric car (Stolz et al. 2016).

1.5 Context and procedure towards global guidance on LCIA indicators

This guidance document is derived from a definition of the audience, the work process that culminated in the workshop, the level of consensus, and the concept that the principles can be supported and defended without requiring absolute consensus among experts. The subsections below address the target audience for the guidance, the status and role of the preparatory work, the list of criteria for recommendations, and the level of consensus.

1.5.1 Target audience

The main target audience of this guidance document are representatives in industry and governments interested in using LCA in strategic planning, environmental management, product improvement, and in setting policies. This target group plays a key role when it comes to commissioning studies on the life cycle-based environmental impacts of products, policies, corporate activities, consumer information, business-to-business communication, etc. The purpose of the guidance document is to allow the representatives to ask for environmentally relevant information related to the environmental impacts of: (1) substances toxic to humans, (2) substances toxic to ecosystems, (3) acidifying and eutrophying substances, (4) land use on soil quality and related ecosystem services, and (5) the use of mineral resources.

Another important target audience of this guidance document are the developers of LCIA methods who have the opportunity to use the latest LCIA framework or implement consensus-based environmental indicators into their current methods. LCIA indicator developers in the field of human toxicity, ecotoxicity, acidification and eutrophication, soil quality and related ecosystem services, and mineral resource use are the third group of individuals and organisations that would benefit from the content of this guidance document.

1.5.2 Status and role of preparatory work

This guidance document draws extensively from the preparatory work performed by larger Task Force groups since the launch of the second phase of the GLAM project in 2016. Each Task Force discussed a specific topic that is reported on in this guidance document and prepared white papers. These white papers formed the background material and the starting point for the week long Pellston Workshop discussions. The preparatory work consisted of:

1. reaching agreement on the exact scope of the environmental indicator being developed. This included the specification of the environmental impacts to be addressed and the LCA-related questions the indicator is supposed to be suitable for;
2. identifying, describing, and evaluating currently available approaches within and beyond the field of LCA;
3. agreeing on one or several candidate environmental indicators that comply with the requirements and are likely to gain acceptance by users;
4. listing the top priority questions and aspects to be discussed and agreed upon during the Pellston Workshop.

The workshop participants based their discussions on these white papers as well as a large number of background reading documents. Though the workshop participants are solely responsible for the recommendations put forward in this guidance document, they acknowledge the invaluable preparatory work laid out by the Task Force members not physically present at the workshop. The achievements reached during the workshop are documented in this guidance document and are expected to form the basis for a series of scientific papers authored by the topical Task Forces.

1.5.3 Criteria for recommendations and level of consensus

The recommendations presented in this guidance document are the result of the consensus-finding process employed throughout the various workshops and consultations. The recommendations are based on supportable evidence, with an aim to ensure consistency and practicality. However, they do not necessarily reflect unanimous agreement and, where necessary, minority views are also included, provided they are rationally grounded and defensible (i.e., based on facts, an underlying basis of argumentation in science, or demonstrated practical application) and are not based on opinion or commercial interests.

When made, these minority views are not given prominence over the more highly recommended approaches (Sonnemann & Vigon 2011).

The body of experts assigned levels of support for a practice or indicator, according to the workshop process, principles, and rules. These levels are stated by consistently applying the terminology of "strongly recommended", "recommended", " interim recommended", and "suggested or advisable". The level of recommendation is determined based on the maturity of the methods, as identified by the following criteria: a) environmental relevance and scientific robustness, b) availability of data / extrapolation approaches within the domain of applicability, c) completeness, d) parsimony, e) documentation and transparency, f) testing, g) stakeholder acceptance and comprehensibility, and h) improvement relative to existing approaches.

Terminology such as "shall" or "should," normally associated with a standard-setting process, is avoided where possible. If such wording is used within a section of the text, the reader is encouraged to consider such use as equivalent to the use of the term recommendation with the corresponding level of support; for example, "shall" is equivalent to "strongly recommended." Interim recommendations are to be applied or used as default (rather than leaving out some inventory flows), while improved methods are being developed and until better factors become available. For some aspects, the experts may not have been able to formulate a clear recommendation. In these instances, either no supportable single recommendation is put forward or various alternatives are presented with no specific recommendation.

1.6 Structure of this report

This report is structured along the topics discussed during the preparation and execution of the Pellston Workshop. Chapter 2 presents an update of the framework and other cross-cutting issues with recommendations on how to address them. Chapters 3 to 7 cover the five topical areas: human toxicity, ecotoxicity, acidification and eutrophication, soil quality and related ecosystem services, and mineral resources. The chapters contain sections documenting the new findings, explaining the recommendations, addressing practicality issues, as well as suggesting and recommending future developments. Finally, Chapter 8 provides an overall synthesis and description of the roadmap toward the development of even more complete global LCIA indicators.

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2. Cross-cutting Issues

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2.1 Scope and overview of issues addressed

Building on the work developed prior to and at the Pellston Workshop in January 2016 (Frischknecht and Jolliet 2016; Jolliet et al. 2018; Verones et al. 2017a), the task force on framework and cross-cutting issues continued its effort to address challenges across multiple impact categories. These efforts are aligned with the need to extend a consistent life cycle impact assessment (LCIA) framework.

The purpose is to ensure that all new developments can be integrated into LCIA in a compatible way, particularly environmental impacts assessed at the endpoint level. To operationalise the framework published by Verones et al. (2017b), several aspects need to be covered in a cross-cutting way:

1. impact pathways within an area of protection (AoP) need to be consistent with each other in order to allow for comparisons across impact categories;
2. the treatment of ecosystem services in the framework and their contributions to different AoPs need to be clarified; and
3. the definition of AoPs related to instrumental values needs further refinements.

Other aspects also need to be covered in a cross-cutting way (e.g., across impact categories and AoPs) in order to enable a consistent connection between life cycle inventory analysis (LCI) and LCIA and to avoid issues, such as double counting impacts. The focus of the cross-cutting task force was to investigate the different aspects that need harmonisation and to derive relevant and robust recommendations.

In recent years, there has been considerable development in LCIA approaches, for example in terms of covered impact pathways, spatial resolution, or consistency for proposed endpoint indicators (e.g., Verones et al. 2017b; Winter et al. 2017; Woods et al. 2017; Mutel et al. 2018). The cross-cutting issues task force appraised all ongoing research efforts, producing new insights and improvements on a number of topics, and provided guidance for further research directions.

Four key topics were brought to the agenda of the second Pellston Workshop:

1. uncertainty assessment and management;
2. the instrumental values framework and the role of ecosystem services;
3. the assessment of ecosystem quality, with specific focus on ecological vulnerability; and
4. the consistent connection between LCI and LCIA.

These four topics were defined after discussion with all members of the task force according to their relevance for further consensus-finding, as well as their level of advancement at the time of the workshop. For each of these key topics, we distinguished between short-term recommendations, i.e., those that can be currently implemented or implemented within the coming 1–5 years, and long-term recommendations or future developments, which are intended to steer further research and development into the desired direction.

2.2 Uncertainty aspects

Uncertainty assessment is largely missing in current LCA practice. In particular for LCIA, the required information is virtually unavailable even at a qualitative level, in contrast to the commonly used pedigree approach for semi-quantitatively characterising different data quality indicators in LCI databases, such as ecoinvent (Weidema et al. 2013). Due to this lack of uncertainty information on characterisation factors (CFs), uncertainty of LCIA results is rarely included in LCA reports and publications. This situation leads to a risk of over-interpretating differences in impacts between compared products or services or mis-prioritising key issues to be addressed.

All LCIA models contain multiple sources of uncertainty, such as parameter uncertainty, model uncertainty, and uncertainty associated with value choices (Hertwich and Hammitt 2001a, 2001b; Huijbregts 1998). The LCIA models recommended in the previous Pellston Workshop (Frischknecht and Jolliet 2016) contained uncertainty information covering some but not all relevant aspects.

For toxicity impacts, several attempts have been made to quantify parameter uncertainty for characterisation results related to certain impact pathways that are chemical-specific (e.g., Fantke and Jolliet 2016). As well as providing a generic, quantitative model uncertainty estimate for characterisation results across chemicals (e.g., Rosenbaum et al. 2008). Additional efforts, made outside the field of toxicity, focused on propagating parameter uncertainty using a Monte Carlo approach (e.g., Roy et al. 2014), combining model and parameter uncertainty (e.g., Henderson et al. 2017), and quantifying impacts of water consumption (e.g., Pfister and Hellweg 2011). However, a consistent procedure for uncertainty assessment is still lacking.

Due to its importance in LCA, uncertainty was already discussed during the previous Pellston Workshop (Frischknecht and Jolliet 2016). The discussion about uncertainty aspects continued throughout the second phase of the flagship project, leading to refinements in the recommendations presented at the Pellston Workshop in 2018. Since 2016, a number of the related recommendations for future research resulting from that workshop have been taken up and further elaborated into the following:

2.2.1 Short-term recommendations

- We strongly recommend that method developers provide sufficient underlying uncertainty information and practitioners evaluate and report uncertainties in impact scores. Making sure to consider the different types of uncertainty (lack of data or contextual knowledge) separately for each impact category, such as input data, model, value choices, and scenarios, as well as the associated variability (inherent data heterogeneity), using the following tiered approach (from low to high level of details), which is aligned with international uncertainty guidance (EFSA et al. 2018; WHO 2014):
  - » *Tier 0, screening, case-generic*: This is the lowest tier and is recommended as the minimum requirement for reporting by practitioners as part of characterisation factors and impact scores. If uncertainty estimates at the level of individual factors or scores are not feasible to be delivered, qualitative generic uncertainty information (i.e., across factors or scores) for each impact category should be provided as an upper estimate (i.e., higher than average uncertainty values across factors or scores), to motivate for more refined analyses of uncertainty in the future.
  - » We additionally recommend that practitioners conduct a hotspot analysis to identify dominating impact(s) and large impact contributions from one or several substances to overall impact scores. Even if uncertainties of these most contributing impact(s) or substances are low, their reduction can lead to overall lower uncertainty when they dominate product-related impact scores. Hence, the identification of such hotspots can assist, once reported back to method developers, in identifying weaknesses and prioritising future data and model improvements. We recommend focusing on the identified hotspots in the reporting of uncertainty by practitioners and, wherever possible, further assessing their related uncertainty in the next higher tier.
  - » *Tier 1, qualitative, case-specific*: The aim of this tier is to refine the case-generic uncertainty values from tier 0. Therefore, better input data quality and data availability need to be provided by method developers, in order to allow practitioners to describe uncertainty, as well as the two sides of the confidence intervals of the uncertainty per source, in a qualitative way. Identified hotspots should then, if possible, be further assessed using a tier 2 approach.
  - » *Tier 2, (semi-)quantitative (e.g., pedigree matrix), deterministic, case-specific*: Information is needed from method developers on the potential ranges of the model input data values per scenario, as well as the sensitivity of the model outputs towards these ranges. The outcome can be variation in output per variation in inputs, limits of confidence intervals, or probability bounds per scenario and uncertainty source. If the impact proves to be a hotspot and it is feasible, we recommend that practitioners carry out further assessment with tier 3.
  - » *Tier 3, quantitative, probabilistic, case-specific*: We recommend this as the highest tier for practitioners to assess uncertainty. It provides the highest level of detail. The prerequisite is that site and scenario-specific information is available from method developers for the distribution of values, as well as their correlations. The resulting uncertainty is characterised in terms of uncertainty and variability distributions for the scenarios, sites, and/or sources.

2.2.2 Recommendations for future developments

- We strongly recommend that software developers provide solutions and/or approaches for enabling systematic, quantitative uncertainty assessments over both LCI and LCIA. These solutions and approaches are recommended to accommodate the uncertainty (reflecting lack of data or contextual knowledge) and variability (reflecting data-inherent heterogeneity) of temporally and spatially differentiated LCIA methods.

» We suggest that method developers explore applicability and limitations of the pedigree matrix approach (Weidema and Wesnæs 1996) to characterise data quality as part of uncertainties in LCIA until better quantification approaches are available.

» We suggest that method developers evaluate the uncertainties associated with "border issues," which refers to artefacts introducing additional uncertainty that arise as a consequence of the selected spatial (or temporal) resolution and associated grid cell dimensions. The framing of grid cells may induce inconsistencies for assessing impacts stemming from sources close to the defined grid cell borders. For example, two very similar and close emission sources that belong to different grid cells, might lead to very different impacts. However, two very different emission sources that are far from each other but within the same grid cells, may lead to similar impacts (e.g., Wannaz et al. 2018). Uncertainties due to inappropriate differences in the characterised impacts from these two sources need be quantified, e.g., in a scenario analysis using different cell dimensions.

» We recommend that method developers explore approaches for assessing uncertainty associated with different levels of spatial, temporal, or archetypal aggregation to identify optimal assessment scales. The uncertainty might arise from either upscaling (increasing spatial, temporal, or any other scale by aggregation) or downscaling (decreasing spatial, temporal, or any other scale by increasing resolution). For example, using different archetypal scales to capture variability in exposure situations (such as indoor, urban, rural) for fine particulate matter impacts, where archetype levels have different levels of associated uncertainty (Fantke et al. 2016b). It is crucial to always distinguish and transparently report variability and uncertainty (e.g., by separately providing confidence intervals for spatial variability and confidence intervals for parameter, model, and/or other uncertainty), since variability (e.g., spatial variability) is inherent to the system and cannot be reduced. Spatial variability is not necessarily part of uncertainty, i.e., it depends on the spatial scale selected in the goal and scope of the study.

» We suggest that method developers explore the possibility of expressing uncertainty results in relation to variability at impact category level, in order to enable the comparability of uncertainty metrics, as well as the comparison of uncertainty results across impact categories. This means that higher uncertainty for a specific impact category is usually associated with a much wider variability range in characterisation results. Whereas, impact categories showing low uncertainty ranges usually show much lower variability ranges in characterisation results. Hence, the relation within each impact category between the uncertainty of individual characterisation results and the variability across characterisation results might be similar across impact categories, which is an important aspect to consider when comparing uncertainty across impact categories.

» We suggest that method developers investigate uncertainty assessment approaches to account for the fact that impact indicators at midpoint level are defined at different locations along the cause-effect chain. More specifically, while some indicators are defined in a way that they are of low environmental relevance (i.e., far from the environmentally relevant endpoint), such as midpoint results for climate change, other indicators are defined in a way that they are of high environmental relevance (i.e., close to the endpoint), such as midpoint results for human toxicity (see Figure 2.1). This way, it would be possible to consider both model-related uncertainties and uncertainty related to results interpretation, such as environmental relevance (Hauschild 2005). This bias in the uncertainties between impact categories may lead to an unfair interpretation if uncertainty assessment across impact categories cannot be performed.

» We suggest that method developers explore ways to systematically account for correlation uncertainty in an LCI-LCIA propagation (e.g., due to correlation between input parameters). The analytical and sampling approaches proposed by Groen and Heijungs (2017) may serve as a starting point in this effort.

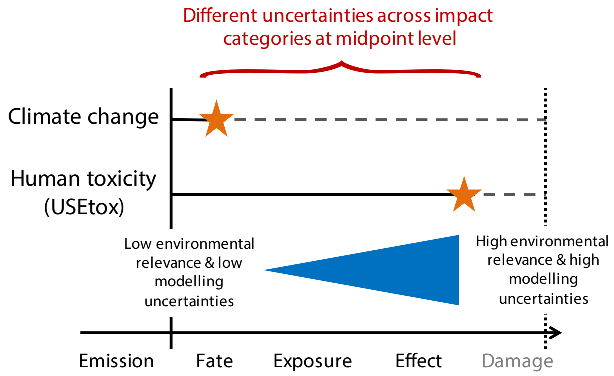

Figure 2. 1. Illustration of different uncertainties across indicators for midpoint impact categories (using the example of climate change indicators defined to be far and human toxicity indicators being defined to be close to the environmentally relevant endpoint for human health damages). Accounting for different extents of uncertainty associated with environmental relevance and modelling uncertainties (inspired by Hauschild [2005]).

2.3 Instrumental values framework

2.3.1 Introduction

Previous studies performed within the Life Cycle Initiative have argued that human health and ecosystem quality should be of concern in LCA because of their *intrinsic* values, whereas natural resources should be of concern because of their *instrumental* and *cultural* values (see Verones et al. 2017b). Intrinsic values represent the values assigned to the existence of an entity itself, i.e., the values inherent to nature independent of human judgement (Díaz et al. 2015). Instrumental and cultural values are defined as being a means to advance human purposes (Zimmermann 2015), thus being the direct and indirect contributions from nature to the achievement of human well-being and quality of life (Díaz et al. 2015).

Besides natural resources, other aspects, such as human capital, biotic and abiotic parts of man-made systems, and ecosystem services can arguably be considered to have an instrumental value for humans. However, with the exception of natural resources, which are addressed in a dedicated AoP (see also Chapter 5), none of the abovementioned aspects (human capital, artificial capital, and ecosystem services) are currently associated with frameworks and operational methods to quantify damages to their previously suggested AoPs. In Chapter 6, an attempt to operationalise ecosystem services (soil quality) is presented. As the only other exception, the Life-cycle Impact assessment Method LIME, a Japanese impact assessment method based on Endpoint modelling, covers damages on artificial capital.

The emphasis here has been on defining a framework to integrate ecosystem services into the general LCIA framework. The development of such a framework is motivated by the need to establish links between the ecological functions and processes, and the benefits to human well-being, in accordance with the goal of establishing ways to deal with instrumental values in LCA.

The term ecosystem services refers to the "ecological characteristics, functions, or processes that directly or indirectly contribute to human well-being, i.e., the benefits that people derive from functioning ecosystems" (Costanza et al. 2017). In addition to several existing definitions of ecosystem services, there are also many different classification systems, systematising ecosystem services, for example, into provisioning (e.g., food and raw materials provision), regulating and maintenance or support (e.g., climate regulation and habitat provision), and cultural services (e.g., recreation, spiritual experience, and sense of place) (Costanza et al. 2017).

To date, damage to ecosystem services is insufficiently covered in LCIA. However, a number of studies have recommended the use of ecological modelling to expand the scope at the level of the LCIA phase (Arbault et al. 2014; Bare 2011; Chaplin-Kramer et al. 2017; Maia de Souza et al. 2018; Othoniel et al. 2016; Liu and Bakshi 2018). These studies suggest that operational models integrating ecosystem services into LCIA are not far from being fully developed. However, as these models are essentially developed for and applied to different contexts such as agricultural systems (e.g., Joensuu and Saarinen 2017), land use (e.g., Bos et al. 2016), or mining (e.g., Blanco et al. 2018), and use different indicators and modelling principles, they do not fit into the suggested LCIA framework in a compatible manner. In addition, life cycle inventory (LCI) data is missing for many potential impact categories dealing with instrumental values.

Some of the challenges developing a comprehensive and integrated cause-effect chain for ecosystem services in LCA, are related to the need to better connect LCI and LCIA (see also section 2.5). The most relevant challenges comprise:

- reaching a consistent definition and delimitation of system boundaries between the technosphere and the biosphere,
- completing and expanding current life cycle inventories to bridge existing gaps and cover all relevant elementary flows,
- developing appropriate impact assessment indicators, making use of the conceptual theories for ecosystem services in LCA (e.g., Cao et al. 2015; Koellner et al. 2013; Othoniel et al. 2016),
- accounting for the interactions among the environmental processes underpinning the provision of ecosystem services (e.g., soil formation might be linked to the total vascular plant diversity).

Since the inclusion of ecosystem services into LCIA is a relatively new and ongoing endeavour, we provide a set of recommendations on how to make further progress with the inclusion of ecosystem services into LCA instead of providing a fixed path. This allows the development of several alternative options in future research.

2.3.2 Short-term recommendations

- We recommend that model developers map ecosystem services according to existing classification systems and identify the connections of LCI and/or LCIA with the mapped ecosystem services. We recommend that model developers select their classification system based on different aspects, such as the distinction between intermediate and final ecosystem services[2], scale of assessment, or the identification of final users or beneficiaries of different services.
- We strongly recommend that model developers outline a detailed LCIA cause-effect chain to connect changes in ecosystem structures and functions, to final benefits and values for humans (cf. Costanza et al. 2017). For example, using the classical "cascade model" (Haines-Young and Potschin 2010; La Notte et al. 2017).
- We suggest that model developers avoid double-counting ecosystem services in models. This means that a distinction between intermediate and final ecosystem services should be made and priority should be given to the final ecosystem services. While the choice of an ecosystem service classification framework and the distinction between intermediate and final ecosystem services can partially aid avoiding double counting, one ecosystem service may still deliver benefits to multiple AoPs, which we do not regard as double-counting. For instance, losses of soil organic carbon (see Chapter 6) may affect human health (via malnutrition) or lead to impacts on ecosystem quality (via biotic production). In a similar manner, consumptive water use (see Frischknecht and Jolliet 2016) also contributes to resources, ecosystem quality, and human health impacts. Thus showing that it is not necessary to aggregate damages into a single AoP. These examples suggest that it is an acceptable practice to not aggregate all impact pathways in a single AoP as long as double-counting is avoided. It is recognized that the AoP "instrumental values" needs further refinement. We recommend that model developers transparently report their cause-effect chains to clarify the pathways to AoPs (damages) and avoid double counting.
- We suggest that model developers transparently report identified synergies and trade-offs that may exist among different ecosystem services, at least in a qualitative way. Through this documentation, practitioners should be made aware of these trade-offs and apply caution when using the models. Regarding trade-offs, the delivery of a specific service, beneficial to human well-being, may, for instance, come along with detrimental impacts to ecosystem quality (e.g., the trade-offs between the benefits from crop production and the impacts on regulating ecosystem services). In a similar manner, synergies may exist among regulation services, with improvement of ecosystem quality and thus, beneficial impacts to human well-being.

2.3.3 Recommendations for future developments

- We suggest that model developers consider different temporal and spatial scales (where and when ecosystem services are generated, and where and when humans benefit from them), for the adequate quantification of ecosystem services, because ecosystem services are provided in a dynamic and inhomogeneous manner, across different space granularity, geographical scope, and time horizons (as in Costanza et al. 2017).

2 Intermediate ecosystem services (ES) are the ecological functions performed by ecosystems that are not directly used by human beneficiaries. They underpin the outputs of final ES, which are the end products of ecosystems, from which humans benefit directly (Fisher and Turner 2008).

When providing the models, practitioners need to be informed about the temporal and spatial scales chosen and differences between different model outcomes. Practitioners, in return, need to transparently report which of the models they use for their study.

- We suggest that model and inventory database developers develop data and metrics based on demand and supply of ecosystem services. This aspect also implies the need to expand life cycle inventories to potentially include information about the provision of ecosystem services with regional information.

2.4 Ecosystem quality: Aspects of vulnerability

2.4.1 Introduction

Impacts on the intrinsic values of biodiversity are assessed under the AoP ecosystem quality. The assessment of these impacts is carried out by globally applicable LCIA models, which, so far, use species richness loss (in terms of "potentially disappeared fractions [PDF]" of species) as a proxy indicator for ecosystem quality. Damages to species richness are assessed with the help of different models, depending on the modelled impact pathway, at local and regional scales. In addition, different impact categories consider different taxonomic groups (or a mix thereof) to generate effect factors for their models.

All current operational models use species loss as the resulting proxy indicator. While their outcomes may appear comparable at first glance, they present fundamental differences, which should be taken properly into account. For instance, some models characterise local species losses, while others characterise global species losses (Woods et al. 2017). The use of the PDF measure in LCA also implicitly presumes that the inhabiting species of all potentially damaged sites are uniform in terms of their vulnerability and do not vary across location. Therefore, the PDF does not reflect that different species and ecosystems may react differently to pressure, as already identified in Frischknecht and Jolliet (2016). The PDF measure should be adapted; it will acknowledge different responses of distinct taxonomic groups or ecosystems to pressure. To adapt it, there is the need to understand and incorporate the aspects of ecological and evolutionary biology that relate the vulnerability of species or ecosystems to stressors (Metzger et al. 2006).

The natural variability in species' vulnerabilities depends on the geographical distribution of the species and related environmental conditions. Therefore, currently estimated local PDF values cannot simply be aggregated according to stressors or over specific areas, nor scaled up to the global level, as vulnerabilities of exposed species and ecosystems vary due to differences in species assemblages that occur due to natural variability at non-disturbed or minimally disturbed reference sites (Zijp et al. 2017). Therefore, as discussed in Verones et al. (2017b), PDF measures using different scales and different taxonomic groups should currently not be combined as such. To facilitate the comparison across impact categories and scales, and to enhance current biodiversity impact approaches to reflect irreversible (permanent) biodiversity loss, Frischknecht and Jolliet (2016) and Woods et al. (2017) recommend including a measure of vulnerability in LCIA (i.e., a vulnerability indicator) to get a vulnerability-adjusted PDF. Such vulnerability-adjusted PDF will reflect the appropriately quantified contribution to potential global damage for a site or region, by including species' and ecosystems' local vulnerability characteristics. By incorporating this information, damages (potential extinctions) are indicated regionally on a basis that can – if needed – be scaled up to a global level. With the scale-up, vulnerability indicators, which are developed using a species-based approach, also give an indication of the vulnerability of the whole ecosystem. The following definitions and recommendations provide guidance towards the development of such vulnerability-adjusted PDF indicators.

The term "vulnerability" has many definitions in ecology (Beroya-Eitner 2016), which makes the incorporation of vulnerability differences in LCIA even more challenging. In the context of LCIA (see also Figure 2.2), we define *ecological vulnerability* as the extent to which an ecosystem, at different levels of organisation (e.g., species, communities, ecosystems), may potentially experience alterations, expressed as potential impacts, resulting from an *exposure* to *environmental stress*. Thereby the *sensitivity* of the ecosystem defines the degree to which potential impacts can affect the ecological properties, processes and functions of ecosystems. When the ecosystem's *adaptive capacity or recovery potential* is not able to compensate for these *potential impacts*, an irreversible (permanent) *damage* may occur. Therefore, two species or ecosystems can have the same *sensitivity* to stress levels, but the final *damage* is co-determined by the *adaptive capacity* or *recovery potential,* so that net damage may be low for one system and higher for another. The latter is then deemed more *vulnerable*. An LCIA approach that enables accounting for vulnerability differences across ecosystems needs to incorporate *sensitivity, adaptive capacity* and *recovery potential* (see glossary for definitions) as key concepts, as all three co-determine potential damage, given species and/or ecosystem characteristics. In addition, adaptive capacity and recovery potential will depend on the type of stressor (pulse or continuous), as they are time-dependent.

We identified adaptive capacity and recovery potential as the key missing components of ecological vulnerability in most existing LCIA methods. Endemism, threat level, and habitat rarity can be used as proxy indicators to incorporate adaptive capacity and recovery potential in LCIA. This is in line with the approach recommended for land use impacts by Frischknecht and Jolliet (2016) and existing "vulnerability scores" in LCIA (Chaudhary et al. 2015; Tendall et al. 2014; Verones et al. 2017a; Verones et al. 2013). Endemism characterises the uniqueness of a species to a defined geographic location and can be seen as an indicator to cover aspects of dispersal ability and immigration ability (see also Figure 2.2).

In addition, functional diversity (i.e., set of functions that organisms perform in a specific level of organisation, such as an ecosystem) is an important aspect to ensure the maintenance of ecosystem functioning, along with functional redundancy (i.e., capacity of

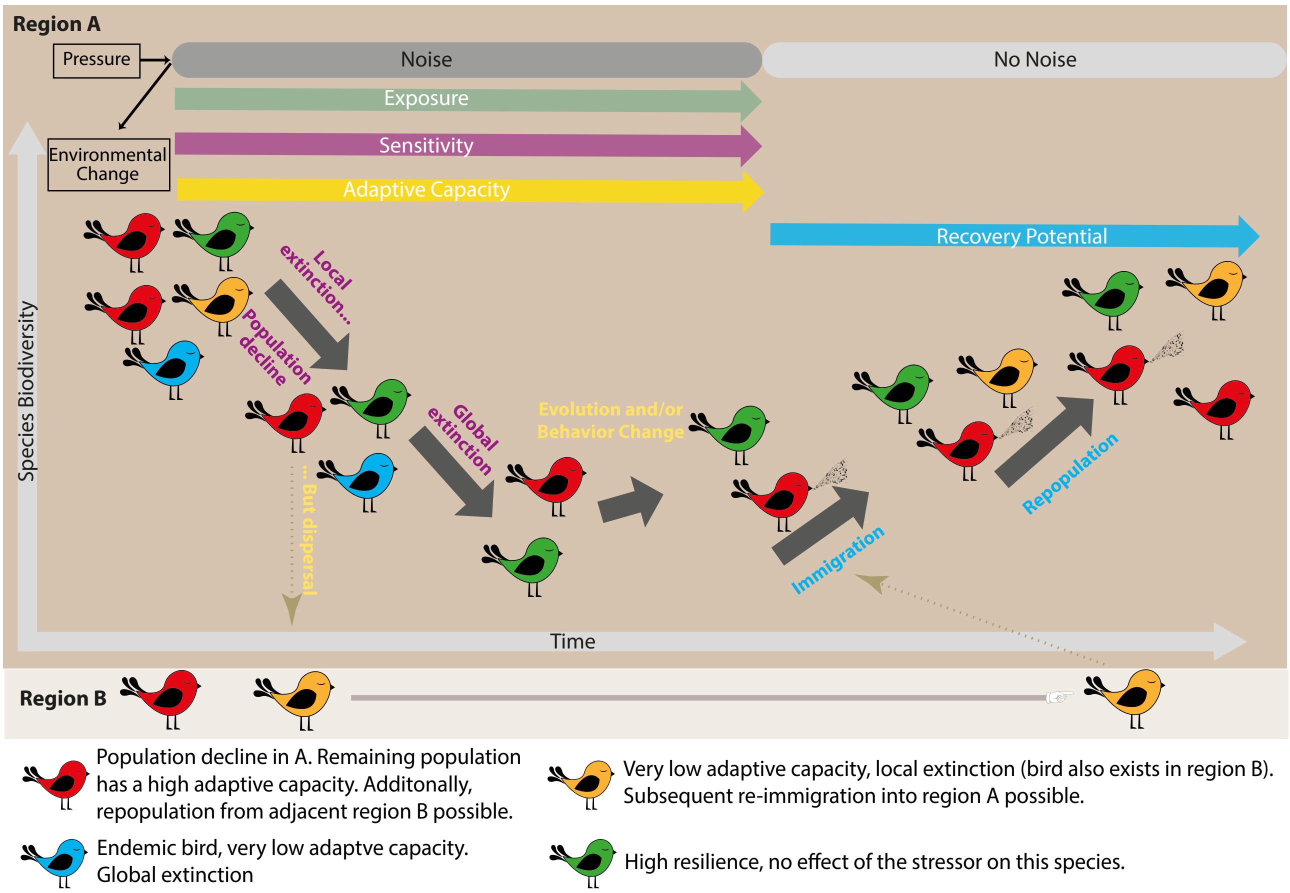

Figure 2.2. Schematic representation of the ecological vulnerability concept.

In the presented example, the stressor 'noise' is causing an environmental change for the four bird species in region A (green box: red, green, yellow, and blue bird). Due to species sensitivity to the stressor 'noise', global (blue bird) and/or local (yellow bird) extinctions may occur. The blue bird is endemic to region A, and, therefore, its extinction in region A represents a global extinction. The yellow bird is not endemic (also lives in region B, orange box) and thus extinction is only local. The green bird is not sensitive to 'noise' and is hence not affected. For the red bird species, a population decline takes place. In addition, the red bird has a high adaptive capacity and changes its behaviour to sing at a higher volume, enabling it to prevent a late local extinction. When the stressor stops, species can recover. This can happen by immigration of species from region B (yellow bird) and/or repopulation of the species in region A (red bird). Species that are globally extinct will not recover (blue bird). This figure shows one of many possible pathways. The species could, for example, also have higher adaptive capacity and low recovery potential or low adaptive capacity but high recovery potential. The arrows (exposure, sensitivity, adaptive capacity, and recovery potential) show during which time span the different elements of the vulnerability concept are relevant (during or after the stressor is active).

organisms to function in a similar manner). Hence, changes in functional diversity and functional redundancy in ecosystems closely relate to long-term vulnerability changes in the system (e.g., a reduction in functional diversity may lead to a higher vulnerable state of that system in the long-term). Further work is needed to explore the options for establishing functional diversity as an additional indicator for ecosystem quality, in addition to the currently used species richness as indicator for intrinsic values. The concepts of ecological vulnerability and functional diversity are both key for understanding ongoing ecological processes and functions.

2.4.2 Short-term recommendations

- We strongly recommend that model developers address aspects of vulnerability with a harmonised approach for all impact categories contributing to the AoP ecosystem quality in order to be able to consistently compare impacts. This consistency in implementation can be achieved, for example, by using the same set of vulnerability aspects (e.g., levels of endemism for all species) that is relevant for the respective impact category (e.g., taking into account that different taxonomic groups are relevant for different impacts or that there are differences in immigration patterns between taxa).
- We recommend that any developed vulnerability scores are added to the impact categories at the end of their impact pathway to translate the local, generalized PDF to global damage. Thus, two sets of CFs might be available from model developers, one that does not consider vulnerability aspects and one that is adjusted for vulnerability.
- We interim recommend the use and refinement of the currently published vulnerability scores (e.g., Chaudhary et al. 2015; Verones et al. 2017a) for further model development. We highlight the shortcoming that these approaches are currently only used by a limited number of relevant impact categories (i.e., land use and water consumption) and for a limited number of taxonomic groups (mammals, reptiles, amphibians, plants, and birds). More coverage in terms of taxa is needed because impacts in different impact categories may be characterised by distinct taxonomic groups. This implies that specific steps need to be taken in the development of the vulnerability scores. In addition, the aggregation across impact categories needs to take the different taxonomic coverages into account.

2.4.3 Recommendations for future developments:

- We suggest identifying several potential additional indicators that could be included in the long-term development of vulnerability scores (amongst others: genotypic diversity, remaining natural land cover, or functional connectivity), and to evaluate and rank them by their potential utility. We suggest working towards including ecological indicators into general and operational LCIA vulnerability scores. For this, we propose investigating the suitability of these indicators to contribute to the vulnerability evaluation system, as well as performing a thorough assessment of additional indicators.
- We suggest addressing the following challenges in future efforts and including these possible indicators into existing "vulnerability scores":
  - » The further development of a consistent framework across relevant impact categories, including consistency across taxonomic groups and in the choice of reference states;
  - » The identification of number and type of indicators that are needed to cover all important aspects of adaptive capacity and recovery potential;
  - » Accounting for possible thresholds (e.g., repopulation cannot occur if only one individual is left). This is also linking to functional redundancy;
  - » And thereby take into account:
    - The availability and reliability of data at a global scale;
    - Potential overlaps and double counting between indicators.

We recommend the development of indicators that unveil the role of organisms on the dynamics and functioning of ecosystems, such as functional diversity (Souza et al. 2013).

2.5 Connecting LCI and LCIA

2.5.1 Introduction

There are on-going initiatives to increase interoperability among different LCI databases including, for example, activities within the Global

LCA Data Access network (GLAD) (United Nations Environment Programme), or the Big Open Network for Sustainability Assessment Information (BONSAI) (Klaja 2015), as well the building of hubs for national databases through the EU Commission's Life Cycle Data Network (LCDN) (Fazio et al. 2016), or the creation of open LCA nexus to host LCI datasets (Ciroth 2013). Initiatives aiming at better data and nomenclature management are also ongoing (Ingwersen et al. 2018; Edelen and Ingwersen 2017; Edelen et al. 2017; Kuczenski et al. 2018). Admittedly, significant progress has been made in the LCA community to increase coverage and accuracy of LCA data in different life cycle stages, however one of the longstanding problems within the LCA community that has received little attention lies in the connection issues between LCI and LCIA phases from a multi-stakeholder perspective. Such issues include (but are not limited to):

- The inconsistency and matching issues in the elementary flows nomenclature.
- The challenges of matching group emissions between LCI and LCIA, including but not limited to:
  1. lack of isomer information, e.g., CFs for propanol emissions versus CFs for propan-1-ol and propan-2-ol;
  2. "undefined" emission or resource flows, such as heavy metals without indication of oxidation state and chemical form, pooling of compounds owing to their affiliation to a specific chemical (e.g., tributyltin hydroxide and tributyltin acetate pooled as tributyltin), resource element extraction without indication of its ore content (e.g., "gold" vs. "gold, 4.9E-5% in ore"), or differentiated land use types (arable land vs. irrigated or non-irrigated arable land);
  3. groups of substances, for which composition varies as function of, e.g., emission sources, like polyaromatic hydrocarbons (PAHs), dioxin or furans, polychlorinated biphenyls (PCB), non-methane volatile organic compounds (NMVOC), petroleum products, etc.
- The ambiguity of defining the boundary between technosphere and biosphere in LCI and LCIA (Rosenbaum et al. 2015; Jolliet et al. 2015) and incomplete modelling, such as near-field exposure related impacts in both LCI and LCIA (Fantke et al. 2016a).
- The incomplete and inconsistent integration of spatiotemporal details in LCI and LCIA (Finnoff and Tschirhart, 2011).
- The different implementation choices in different LCA databases and software packages, resulting in different results for a same inventory (Speck et al. 2015; Herrmann and Moltesen 2015).

These challenges can undermine the reliability of LCA results and should therefore be addressed consistently across the broad spectrum of LCI data and impact assessment models. In that setting, we build on a comprehensive review of these inconsistencies and gaps to provide short-term and long-term recommendations for improving the connection between LCI and LCIA. The targeted audiences for this recommendation are LCI database developers, LCIA method developers, LCA software developers, and international multi-stakeholder governance bodies, such as the Life Cycle Initiative (where relevant, the targeted stakeholder groups are specified in below recommendations).

2.5.2 Short-term recommendations (including important or urgent and relatively easy to implement)

- **Establish an international, multi-stakeholder collaborative structure.** We recommend a collaborative effort to be formed, preferably under the auspices of the Life Cycle Initiative, to build consensus and harmonisation on central topics related to LCI and LCIA connection and data exchange (see Figure 2.3). Therefore, this effort needs to go beyond current initiatives (e.g., GLAD or LCDN), which focus on specific topics (e.g., nomenclature harmonisation) and adopt a multi-stakeholder approach to engage the developers of LCI databases, LCIA methods, and LCA tools through a stable multi-stakeholder governance entity. This governance entity shall facilitate stakeholder engagement in consensus building processes and ensure consistency and compliance checks. Its scoping is intended to capture the following aspects:
  - » Data transfer format(s)
  - » Nomenclature for elementary flows (e.g., "carbon dioxide"), associated properties (e.g., biogenic), and specifications (emission compartment "air, high population", or geographical coordinates)
  - » Linkage between LCI and LCIA, e.g., interface between LCI and LCIA models
  - » Implementation of LCI and LCIA data in a

consistent way in LCA software with transparent documentation

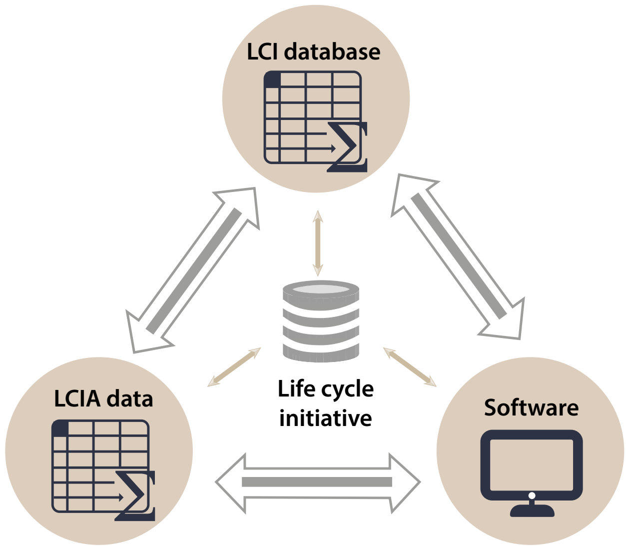

Figure 2.3. Proposed international, multi-stakeholder collaborative structure for facilitating harmonisation in LCI and LCIA connection and data exchange

- **Support for LCIA method implementation.** We strongly recommend that a joint effort is formed to support the task of mapping and implementing LCIA methods into various LCA databases, software, and tools. This may be nested within the collaborative structure (see Figure 2.3). An open dialogue between the LCA software and tool developers and the LCIA method developers is recommended for checking and reporting the consistency of results when implementing LCIA methods (potentially including selection and recommendation of LCIA methods). We recommend transparent documentation of the implementation, including versioning and changes being made (as suggested in the last Pellston report [Frischknecht and Jolliet 2016]).
- **Common data exchange format.** We strongly recommend that all stakeholders build consensus on a common data exchange format to facilitate data transfer, e.g., from LCIA modeller to LCA software. This format is required to account for evolving needs from the LCI and LCIA methods side, such as spatiotemporally differentiated impact methods, and to ensure better documentation of spatiotemporal information. Until now, LCI databases (ecoinvent, Gabi, ELCD, EU EF-compliant data, Japan IDEA, US LCA Digital Commons) use a variety of data exchange formats. However, CFs are often provided in many different ways incompatible for data exchanges. A consensus around a common data transfer format, such as comma-separated values (CSV), will facilitate data exchanges and avoid inconsistencies or errors during implementation by different LCA software developers.
- **Common reference nomenclature and classification system.** We strongly recommend that all stakeholders support and develop a common reference nomenclature and classification system, for specifying names of elementary flows, classifications (e.g., to distinguish chemical classes and compartments), and associated properties (e.g., technical, chemical, or economic flow properties). A nomenclature and classification system has an evolving nature, which in principle can be developed at the lowest level of detail, so that the differentiation within the classifications can be seen as an aggregate of two or more of this evolving base nomenclature (e.g., indoor air emissions consist of household indoor and industrial indoor emissions). Until such a common unique nomenclature system is developed, we recommend that stakeholders follow one of the existing nomenclature systems, or as a minimum provide, clear descriptions of the used nomenclature.
- **Identifying and harmonising most relevant elementary flows.** We suggest identifying and harmonising discrepancies in LCI and/or LCIA for the most significant and relevant elementary flows. A prioritisation needs to be performed for listing elementary flows and corresponding characterisation factors associated with large impact contributions for each impact category, and also identifying significant elementary flows that have no corresponding LCIA characterisation factors, and vice versa (e.g., frequency analysis of an elementary flow being used in a LCI database or expert judgement). Care should be taken in this process to account for the dependence of the flow relevance or significance on the type of systems or sectors, hence ensuring that no flow that is potentially significant or relevant to a type of system or sector is left out.
- **Handling of group emissions.** We strongly recommend that LCIA method developers provide CFs for groups of substances based on default substance group compositions or emission source archetypes (e.g., applicable to cationic metals). Where this is not applicable, LCI modellers are

recommended to differentiate group emission flows based on emission source types, substance properties, and/or receiving environment (e.g., differentiating and reporting pesticides as individual active ingredients). We recommend this differentiation is done with (i) uncertainty quantification, (ii) harmonisation across LCIA methods, and (iii) harmonised flow nomenclature across LCI and LCIA.

- **Spatiotemporal differentiation and archetypes**. We complement the recommendation made at the previous Pellston Workshop (Frischknecht and Jolliet 2016) about spatial data mapping. We recommend that developers of LCI databases, LCIA methods, software, and tools (and not just LCIA method developers) use a standardised format for documenting and reporting regionalised data. Such standards are recommended to follow the Open Geospatial Consortium (OGC 2016), see Chapter 2 of Frischknecht and Jolliet (2016). When more detailed spatial information is not available for either LCI or LCIA, a suggested solution is to develop regionalised (e.g., archetypes used for particulate matter impact assessment in Fantke et al. [2017]) or sector-specific (e.g., differentiation between agricultural and non-agricultural sources for eutrophication; see Chapter 3 of this report) archetypes by differentiating key properties that have substantial influence on impact quantification. We strongly recommend that the variability of aggregated numbers in archetypes as an indication of improvement potentials, are reported when deciding to go for spatially and temporally explicit assessments (Mutel et al. 2018).
- **Clear interface and complete coverage between LCI and LCIA model.** We strongly recommend that the boundary between LCI and LCIA, i.e., between emission or resource flow inventory and point of departure of the fate model, is harmonised and transparently described for both LCI and LCIA modelling at the level of substances or groups of substances. That way, LCI and LCIA models can be linked without gaps or overlaps, which removes any ambiguity. Such an alignment has been made for pesticides (Rosenbaum et al. 2015). Remaining issues to consider for harmonisation include the use of fertilisers on agricultural soil, and the handling of consumer and worker exposure to chemicals. If the LCI reports the mass of chemicals applied or used in the product, the mode of application should be specified together with the flows (Jolliet et al. 2015).

2.5.3 Recommendations for future developments:

- **Nomenclature harmonisation.** To complement the abovementioned short-term recommendation to harmonise the nomenclature of most significant flows (i.e., following the prioritisation step), we suggest that all elementary flows become harmonised.
- **New elementary flows**. We suggest developing guidance to assist LCI and LCIA method developers when a new elementary flow is required, albeit not existent in current nomenclature systems.
- **Handling "unspecific" flows or classification**. We strongly recommend further differentiating unspecified flows (e.g., differentiating land use management practice, water emitted to the rest of the world, etc.)
- **Improving flexibility and efficiency of LCA software to handle spatiotemporally differentiated computation.** LCA software or tools face challenges to efficiently address increased level of details, especially those from spatiotemporal differentiations and archetypes (including additional sub-compartments or subcategories, such as emission heights for particulate matter), in LCI datasets and LCIA methods. We suggest developing more flexible modelling frameworks and features, such as coupling with Geographical Information Systems (GIS), to incorporate the spatiotemporal resolution at different scales within the calculations.

2.6 Normalisation references

Following Pizzol et al. (2016) and the recommendations from the last Pellston Workshop (Frischknecht and Jolliet 2016), research is underway to determine global normalisation references for the impact categories addressed in this report, aligning them with normalisation references for LC-IMPACT (Verones et al. 2019), Impact World+ (Bulle et al. 2019), and ReCiPe2016 (Huijbregts et al. 2017) LCIA methodologies, i.e., use of same normalisation inventory and reference year. Different inventory approaches, for instance using process-based data through a bottom-up approach to complement commonly-applied top-down approaches based on nation-wide environmental databases, should be considered.

Beyond their use in practice, the normalisation references can be used to check the developed LCIA methods by evaluating the plausibility of the global damage results, e.g., whether or not the order of magnitude is realistic, in comparison with that of other global damage assessments (e.g., normalisation references derived for other LCIA methodologies). Potential biases and uncertainties in the results should be considered in such check, including the misaligned coverage of substances across the normalisation inventory and the set of characterisation factors and specific uncertainties associated with the determination of global emissions or resources from incomplete data (Heijungs et al. 2007; Laurent et al. 2015; Benini and Sala, 2015; Sala et al. 2015).

2.7 Other aspects

2.7.1 Addressing positive effects

Negative characterisation factors may be developed for specific substances in some impact categories, due to potential positive effects on the considered AoP. This may, for example, occur in human toxicity impact assessment where exposure to essential metals might be beneficial for the population fraction that is deficient in these metals, or for certain pharmaceuticals (Debaveye et al. 2018). There might also be a potential increase in species richness from increased loading of nutrients or acidifying substances (see Chapters 3-5). In those situations, the derivation of effect factors from dose-response curves may be associated with negative slopes, hence yielding negative effect factor values (and negative characterisation factors, possibly indicating a benefit).

As part of the recommendations from the previous Pellston Workshop, we reiterate the recommendation to practitioners to report both positive and negative impacts separately to ensure transparency, while allowing summation to an aggregated indicator score. We additionally recommend LCIA method developers to document potential occurrences of positive effects associated with specific substances and/or environmental processes, and to explicitly report the inclusion or exclusion of these positive effects in the derivation of characterisation factors.

2.7.2 Model evaluation

It is important to ensure that LCIA results reflect the actual environmental mechanisms as far as possible. We therefore recommend that LCIA method developers ensure the underlying models that support development of LCIA characterisation models are evaluated as much as possible (e.g., via comparison with other models or measurements wherever possible), and to test and evaluate their proposed LCIA characterisation models to the extent possible (e.g., through use of normalisation; see Section 2.6, including consideration of biases and uncertainties associated with the normalisation inventory). We recommend that LCA practitioners evaluate their case study system models and ensure consistency across LCI-LCIA (see Section 2.5). These evaluations can be facilitated if models and results are transparently documented, according to the recommendations in issued in the previous report (Frischknecht and Jolliet 2016). Ensuring consistency across LCI-LCIA and full model evaluation might be difficult; especially when involving confidential data, which cannot be evaluated at times. For a detailed discussion about data confidentiality, please see Section 4.3.2.

2.7.3 Reporting and harmonisation

As a reiteration of a generic recommendation from the previous Pellston Workshop (Frischknecht and Jolliet 2016), we also stress the importance of transparent reporting in LCIA model development and LCA case studies (e.g., assumptions made, obtained LCIA results, and interpretation). We do not provide new recommendations regarding transparent reporting but urge the reader to check and follow the guidelines previously published (Section 2.5 in Frischknecht and Jolliet 2016). Moreover, we strongly recommend ensuring harmonisation between LCIA models and LCI datasets, for example using comparable reference states and harmonised approaches for working points (for the derivation of damage factors) for different impact categories in the different AoPs.

2.8 Summary

The task force on framework and cross-cutting issues strives towards better harmonisation, transparency, and compatibility within LCIA and across LCI-LCIA, as well as in LCA case studies and their interpretation. The recommendations made so far point to this direction in order to satisfy the ultimate goal of contributing to more robust and informed decision-making. However, the harmonisation efforts are far from being finished and research needs and efforts for several aspects are identified (non-exhaustive list).

- Finish the ongoing development and integration of means to perform systematic and comprehensive uncertainty assessment in LCA case studies. This requires methods for holistic uncertainty assessments throughout the LCI and LCIA phases, as well as LCA software capacity to handle such assessments.
- Investigate options to expand the assessment of impacts on biodiversity by integrating other measures than species richness into LCIA modelling (e.g., functional diversity).
- Develop operational indicators to account for ecological vulnerability aspects.
- Identify the links between ecosystem services and the dedicated AoP for instrumental values by means of operational models. It must be taken into account that ecosystem services may be linked to and aggregated under different AoPs.
- Develop guidance to standardise the way aggregation across spatial scales is handled (e.g., aggregating primarily on watersheds prior to aggregating on country levels or vice versa) and standardise ways to calculate confidence intervals.
- Take the temporal dimension of impacts into consideration, such as temporally differentiated emissions, temporary storage, and delayed emissions, as well as the seasonality in LCI and LCIA models. A differentiation over time of the impact results can be considered by LCA practitioners in their interpretation and communication of case studies.
- Agree on a governance body for disseminating, implementing, and maintaining the recommendations being made by this initiative (such as shared nomenclatures, data transfer format, and linkages between LCI and LCIA) as shown in Figure 2.3. We suggest the Life Cycle Initiative takes the lead on this process.
- Work further on updating and harmonising the LCIA framework, in order to cover all aspects (including instrumental values) in a holistic manner.

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3. Acidification and Eutrophication

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3.1 Scope

This chapter provides guidance towards consensus in modelling approaches and indicators that capture impacts from acidification of terrestrial systems and eutrophication of freshwater and marine systems. Terrestrial acidification is the change in soil chemical properties (e.g., decrease in soil pH, decline in base saturation) caused by the inputs of and dissociation of compounds with acid-base chemistry, such as oxides of sulfur or nitrogen. Aquatic eutrophication is the process that begins with the delivery of nutrients (largely nitrogen and phosphorus) to ecosystems, promoting the growth of nutrient-limited species, which has the potential to drive a cascade of changes, including a decrease in dissolved oxygen. If the inputs of acidifying or eutrophying substances exceed the capacity of ecosystems to assimilate these inputs, there may be changes in habitat, species composition, and ecosystem functions (Hassan et al., 2005).

Life cycle impact assessment (LCIA) approaches for the characterisation of acidification and eutrophication aim to trace the fate of an acidifying or eutrophying emission, the degree to which a sensitive environmental receptor is exposed, the effect of that exposure, and the severity of the effect. Despite substantial recent efforts to capture these impact pathways more fully in LCIA, no clear consensus exists on the use of a specific impact indicator, and some LCIA methods that do not account for fate and lack effect modelling are still in use. This variability in modelling approaches limits the comparability of results from different studies, creating a need for global consensus recommendations. This guidance addresses current environmental concerns: recently, 11% of global vegetation was receiving acidifying inputs in excess of critical loads (Dentener et al. 2006), and emissions of acidifying substances have increased in Asia and Africa, despite decreasing in Europe and North America (Vet et al. 2014); application of P fertilizer and creation of reactive N are estimated to be greater than twice the proposed planetary boundaries (Steffen et al. 2015).

The recommendations presented in this chapter use current state-of-the-art LCIA as a point of departure; we aim to balance the representation of physical, chemical, and biological processes with parsimony in modelling. Recommended approaches are commensurable with other ecosystem impacts, such as ecotoxicity or land use, in order to allow for comparison of ecosystem damage resulting from different stressors. The recommended framework is applicable on a variety of spatial scales and includes global default values. Recognising that LCIA models for acidification and eutrophication benefit from models in other disciplines, we also briefly provide recommendations for further improving eutrophication and acidification modelling in LCIA. While there is ongoing work to improve modelling of acidification of aquatic systems and eutrophication of terrestrial systems (Azevedo et al. 2015; Midolo et al. 2019; Posch et al. 2019), the mandate of this task force was to address acidification of terrestrial systems and eutrophication of aquatic systems.

3.2 Impact pathway and review of approaches and indicators

3.2.1 Acidification

Substances with acid-base chemistry may contribute to the acidification of terrestrial and aquatic systems, reducing base cation supply or increasing proton (H^+) supply (Figure 3.1; Norton and Veselý 2003). This chapter focuses on terrestrial acidification due to emissions to air, although Figure 1 shows a variety of impact pathways for comprehensiveness. Oxides of sulfur or nitrogen, as well as ammonia, are the most important anthropogenic contributors to terrestrial acidification (Bouwman et al. 2002), and therefore are the focus of this work. Their reactions in the atmosphere may produce acidifying substances or redox-active substances, whose further products may release H^+, deposit onto land or vegetation surfaces, and eventually make their way into the soil system (Norton and Veselý 2003; van Zelm et al. 2015; World Health Organization 2006).

The extent to which ecosystems are buffered against inputs of acidifying substances depends on the state of the receiving system, which varies in space and time (Blaser et al. 1999; Clair et al. 2007; Dangles et al. 2004). Underlying geology plays a major role in susceptibility to acidifying inputs; as areas with carbonates or silicates containing iron and magnesium may release base cations that potentially counteract acidification processes (Norton and Veselý 2003). Effects of acidification include changes to nutrient regulation by terrestrial ecosystems, with effects ranging from loss of biomass to competitive exclusion by acid-tolerant species (Falkengren-Grerup 1986; Roem and Berendse 2000; Zvereva et al. 2008). Likewise, deposition of acidifying substances may mobilize Al^{3+}, a substance that is toxic to most plants and aquatic organisms (Driscoll 1985; Poschenrieder et al. 2008).

3.2.2 Eutrophication

Eutrophication refers to the process that begins when ecosystems receive excess inputs of limiting nutrients (typically nitrogen or phosphorus) (FAO 2018; Schindler 2006; Vitousek et al. 1997; Vollenweider 1968). This chapter focuses on eutrophication in aquatic (freshwater and marine) systems. If the input of limiting nutrients to an aquatic system exceeds the capacity of that system to assimilate those nutrients, ecosystem structure and functioning may change via the growth of phytoplankton, change in plant composition in the photic zone, alter predator-prey relationships, result in changes in habitat and respiration of organic matter, and cause reduction in dissolved oxygen concentration in the water column (Figure 2; note that for comprehensiveness, Figure 3.2 shows impacts to terrestrial systems as well).

While eutrophication does occur naturally, LCIA models focus on connecting emissions from anthropogenic sources such as synthetic fertilizers, manure, sewage, and treated wastewater and related sludge to eutrophication impacts. Dominant contributors to eutrophication impacts are inorganic P and N compounds: phosphate (PO43-), NH3 or NH4+ (ammonia and ammonium), NO3- (nitrate), and gaseous nitrogen oxides (NOx) (Henderson 2015). In current LCIA practice, nitrogen is assumed to be the limiting nutrient in marine systems, while phosphorus is assumed limiting for freshwater. These assumptions have been driven by modelling parsimony, however, co-limitation of nitrogen and phosphorus may occur in both systems, and other substances, such as silica, may be limiting as well (Azevedo et al. 2015; Bouwman et al. 2009; Carpenter et al. 1998; Elser et al. 2007; FAO 2018; Garnier et al. 2010; Howarth and Marino 2006; Payen and Ledgard 2017; Schindler 2006).

3.3 Process and criteria applied to select the indicator(s)

There have been model comparison efforts conducted before (Hauschild et al. 2013; JRC-IES 2010b; Margni et al. 2008), but these have been restricted to recommendations for a specific area of the world (e.g., Europe). Therefore, there is a need to provide global guidance to practitioners on terrestrial acidification and aquatic eutrophication. In this work, conducted through monthly meetings with global membership, the following methods (and underlying models) for acidification and eutrophication were assessed:

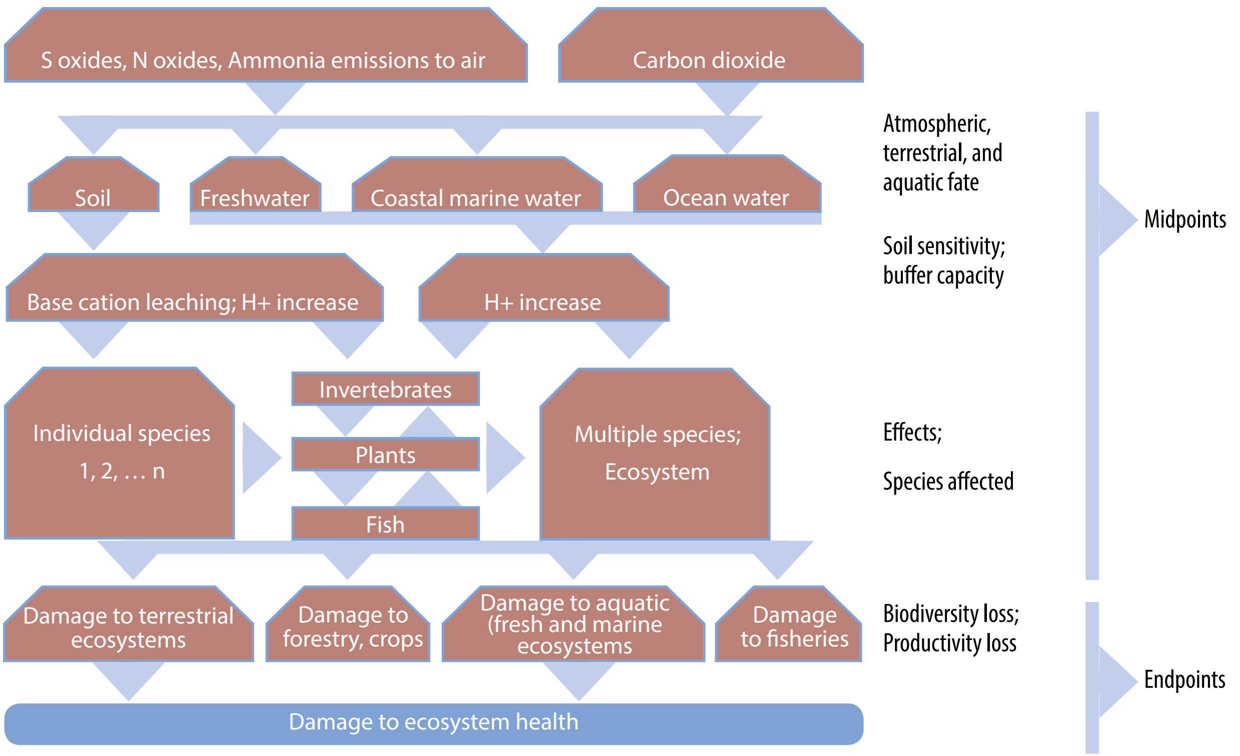

Figure 3.1. Impact pathway for acidification (van Zelm et al. 2015, adapted from JRC-IES 2011). Not all pathways shown are captured in the recommended LCIA framework.

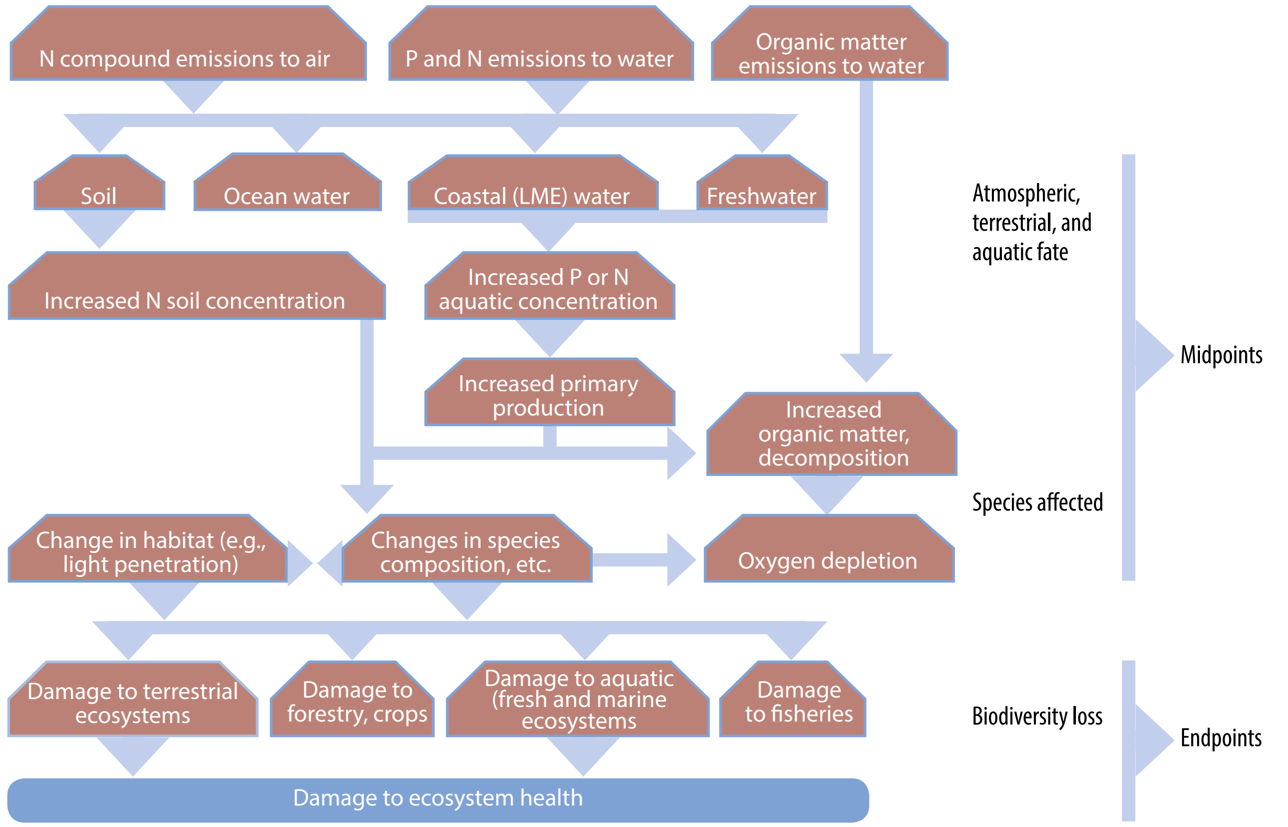

Figure 3.2. Impact pathway for eutrophication (Henderson 2015, adapted from EC-JRC 2010a). Not all pathways shown are captured in the recommended LCIA framework.

- Accumulated Exceedance (Seppälä et al. 2006)
- CML 2002 (Guinée et al. 2002)
- EDIP 2003 (Hauschild and Potting 2005; Potting and Hauschild 2005)
- IMPACT 2002+ (Jolliet et al. 2003)
- IMPACT World+ (Bulle et al. 2019)
- LC-Impact (Verones et al. 2016)
- ReCiPe 2008 (Goedkoop et al. 2013, 2009)
- ReCiPe 2016 (Huijbregts et al. 2017, 2016)
- TRACI (Bare et al. 2003; Norris 2003)

In the case of the IMPACT and ReCiPe methods, changes to the acidification and eutrophication models were not revisions of previous models but additions of new models, bringing conceptual changes to the LCIA method. Thus, previous and updated versions of these models were included in the assessment. Other models were judged to be superseded or lacking sufficient documentation for comparison[3]. The group applied criteria by which to qualitatively assess models and methods; these criteria were consistent with those applied in the first phase of the flagship project (Frischknecht and Jolliet 2016). The environmental relevance criterion was adapted as described below.

Consistent with the flagship project goals, it is desirable to have a globally relevant model. Because of the high spatial variability of acidification (Potting et al. 1998; Roy et al. 2012a) and eutrophication (Helmes et al. 2012) impacts, approaches that provide spatial differentiation are preferable. These two criteria created a clear means to identify models for further consideration in this process (i.e., IMPACT World+, LC-Impact and ReCiPe 2016). Other methods lack mechanistic or empirical fate and effect modelling, global coverage, or spatial differentiation[4]. Specific issues related to fate and effect are described in Section 3.5. With respect to emissions coverage, models that included the substances identified above were prioritised: for acidification, SOx, NOx, and NHx; for eutrophication PO43-, NHx (aqueous or gas-phase), NO3- (aqueous), and NO_x (gas phase).

3 Eco-indicator 99 (Goedkoop and Spriensma 2000), EDIP 97 (Wenzel et al. 1997), EPS 2000 (Steen 1999a, 1999b), LIME (Itsubo and Inaba 2003), LUCAS (Toffoleto et al. 2007), MEEuP (Kemna et al. 2005), Swiss Ecoscarcity 07 (Frischknecht et al. 2009)

4 For example, CML 2002 (Guinée et al. 2002) is site-generic. Other methods consider fate and provide spatial differentiation of characterisation factors but are limited to specific regions, such as Europe (Eco-indicator 99 [Goedkoop and Spriensma 2000], EDIP2003 [Hauschild and Potting 2005], ReCiPe 2008 [Goedkoop et al. 2009, 2013]), North America (LUCAS [Toffoleto et al. 2007]), or the US (TRACI [Bare et al. 2003]).

Depending on the position along the impact pathway (Figures 1 and 2), characterisation factors (CFs) can either be derived at a midpoint or endpoint level. Since both types of indicators are useful depending on the decision context (Rosenbaum et al. 2018), the task force recommends that both midpoint and endpoint CFs be provided for acidification and eutrophication. In keeping with the current and the preceding volume (Frischknecht and Jolliet 2016), the recommended LCIA damage endpoint is Potentially Disappeared Fraction (PDF) of species.

3.4 Description of indicator(s) selected

This section presents the recommended indicators, while the level of recommendation is further discussed in Section 3.8.

- For freshwater eutrophication, the indicator at midpoint level measures freshwater eutrophication potential in phosphorus equivalents (Peq) based on the fate model of Helmes et al. (2012). The CFs at endpoint level measure damage (PDF.m3.yr) to freshwater ecosystems based on the fate above plus inclusion of effect of total P changes on autotrophs, aquatic invertebrates, and fish from Azevedo et al. (2013a).
- For marine eutrophication, the midpoint indicator measures eutrophication potential in nitrogen equivalents (Neq) based on Cosme, Mayorga et al. (2017). At endpoint level, CFs measure damages (PDF.m3.yr) to benthic ecosystems for six heterotrophic taxonomic groups across five climate zones, based on Cosme, Jones et al. (2017).
- For terrestrial acidification, the midpoint indicator expresses acidification potential in SO2 equivalents (SO2eq) based on Roy et al. (2012b). The endpoint level CFs measure damage (PDF.m2.yr) to terrestrial ecosystems for vascular plants across 13 biomes based on the midpoint, plus soil sensitivity and effect assessment according to Azevedo et al. (2013b) and Roy et al. (2014).

Note that endpoint indicators do not consider species vulnerability or resilience (see Chapter 2, crosscutting issues, for discussion of additional ecological indicators).

The recommended CFs are based on the same underlying models as those used by IMPACT World+ (Bulle et al. 2019), LC-Impact (Verones et al. 2016), and ReCiPe 2016 (Huijbregts et al. 2016). However, the recommended CFs differ with respect to aggregation. Emissions of acidifying and eutrophying substances may be associated with agricultural processes (e.g., fertilizer application) or non-agricultural processes (e.g., combustion for energy or sewage discharge). Therefore, we provide three sets of aggregation to country or global levels for different types of activities: agricultural, non-agricultural, or generic. Furthermore, where possible, effect factors are based on current environmental conditions, as discussed below.

3.5 Model, method, and specific issues addressed

3.5.1 Freshwater eutrophication

For freshwater eutrophication, the fate factor predicts the increase in phosphorus in a freshwater system due to an emission to freshwater. The effect factor relates P concentration to species disappearance, although the mechanisms that lead to eutrophication are not fully captured in LCIA models (see Section 3.2.2 and 3.5.4).

Fate

The recommended fate model (Helmes et al., 2012) accounts for the advective transport and removal of dissolved, inorganic P through water withdrawal and retention (settling after uptake by biomass or adsorption to suspended solids in waterways). The underlying hydrologic data for Helmes et al. (2012) is based on a digital elevation model with reconciled grid discharge at a resolution of 0.5° x 0.5° (Fekete et al. 2002; Vörösmarty et al. 2000a, 2000b). Higher resolution datasets are becoming available (Lehner and Linke 2015), and future modelling should include updated hydrologic data.

While the P fate model is adequate at present, limitations such as the following and those noted in Section 3.5.4 A need to be addressed in the future. Of necessity, Helmes et al. (2012) adjust lake and reservoir grid cell water volumes, but future hydrological datasets may obviate the need for such adjustments. Sewage treatment removal of P is not included in the model, which can lead to an overestimation of P transport for flows passing through urban centers. Furthermore, evaporation is not included in irrigation, nor does the model account for the transfer of P from agricultural soil to freshwater.

Exposure

Currently, exposure is not modelled for freshwater eutrophication, as models do not account for P speciation and explicitly model particulate, dissolved, and biotically bound P species. Once fate models include P speciation more fully, it is recommended that exposure be considered in future work.

Effect

The selected model is based on the relationship between relative species richness (RSR) and total phosphorus (TP) concentrations (Azevedo et al. 2013a). Damages are quantified by the potentially not occurring fraction (PNOF) of species. (See Section 3.5.4 for a discussion of the relationship of PNOF to PDF.) The model differentiates cold, temperate, xeric, and sub/tropical climate regions and two kinds of water bodies: lakes and streams. Species captured in the model include cyanobacteria, algae, macrophytes, invertebrates, and fish. The effect factor (EF) is calculated by means of the logistic regression of the patterns of the TP and RSR and the slope at the point where the RSR decrease equals 0.5. The dataset is based on spatially explicit data and is collected from the peer-reviewed corpus (Azevedo et al. 2013a).

3.5.2 Marine eutrophication

Recent developments by Cosme and colleagues (Cosme and Hauschild 2017, Cosme, Jones et al. 2017, Cosme, Mayorga et al. 2017, Cosme and Hauschild 2016, Cosme et al. 2015) are the first in the LCA literature to attempt to characterise marine eutrophication impacts by accounting for fate, exposure, and effect in the marine compartment. Furthermore, the model has global coverage and is spatially explicit at the resolution of freshwater basins and large marine ecosystems (LMEs). The task force recognises the important contribution that this work represents. However, as this impact category and the models of Cosme et al. have not yet been used in many LCIA studies, the task force also emphasizes the importance of continued evaluation and improvement of models for this impact category.

Fate

Cosme, Mayorga et al. (2017) developed spatially explicit fate factors (FFs) for nitrogen emissions to soil, freshwater, and coastal marine systems. For soil and freshwater, fate factors for dissolved inorganic nitrogen (DIN) are based on an application of the Global Nutrient Export from WaterSheds 2 (NEWS 2) model (Mayorga et al. 2010). NEWS 2 estimates nutrient emissions to regional and global surface waters. NEWS 2 is a steady-state hybrid (mechanistic and empirical) watershed model that provides annually averaged dissolved organic and inorganic nitrogen, phosphorus, and carbon, and particulate nutrient emissions to major river basin outlets globally, including endorheic and coastal waters. Within NEWS 2, dissolved nitrogen and phosphorus species at the watershed outlet can be sourced to landscape (soil) emissions, atmospheric (for N only), agricultural, and human waste and sewage. Inputs to the model are at a 0.5° x 0.5° grid scale; however, these are aggregated to the basin (watershed) scale.

For marine emissions, residence time in LMEs is modelled as a function of advection and denitrification. As noted in the sensitivity analyses of Cosme, Mayorga et al. (2017), the residence time in the LMEs is an important parameter in the model, but robust estimates of this parameter are not available.

Exposure

Cosme et al. (2015) introduce an exposure factor (XF) for marine eutrophication to provide a mechanistic model for ecosystem responses and to predict distinct impacts due to nutrient exposure in coastal marine zones. The XF translates N inputs to surface waters to a reduction of O_2 in benthic waters. This model takes into account primary production, metazoan consumption, and bacterial degradation in benthic waters. Oxygen consumption results from the degradation of algal biomass, the production of which was estimated based on Redfield stoichiometry, creating spatially explicit exposure factors for 66 coastal LMEs under five climatic zones (polar, subpolar, temperate, subtropical, and tropical). Typically, exposure factors estimate a bioavailable fraction of the emitted substance. Here, the XF translates an inventory flow (DIN input) into a variation of another substance (oxygen consumption) in the receiving ecosystem. This approach is necessitated by the complexity of the impact pathway, since nitrogen on its own does not cause an effect on exposed species.

While the model accounts for the persistence of nitrogen in surficial marine waters, and respiration in benthic waters, the model does not yet account for the potential replenishment of oxygen in those systems. Oxygen may be replenished via advection or diffusive transfer, offsetting consumption via respiration of organic matter. This task force has not assessed the magnitude of this potential discrepancy.

Effect

Effect factors convert levels of oxygen depletion into Potentially Affected Fraction (PAF) of species. Cosme et al. (2016) use a mixture of laboratory and field hypoxia sensitivity thresholds from the literature for several taxonomic groups (fish, crustaceans, mollusks, echinoderms, annelids, cnidarians) across five climatic zones to estimate effect factors expressed as (PAF). m^3/kgO_2. (See Section 3.5.4 for a discussion of the relationship of PAF to PDF.)

3.5.3 Terrestrial acidification

The cause-effect chain for terrestrial acidification translates emissions of acidifying substances to intermediate reaction products or impact indicators (H^+ and soil pH, respectively), which are then linked to damages. In the recommended model, these damages represent the change in relative loss of terrestrial vascular plant species due to an emission change of nitrogen oxides (NOx), ammonia species (NHx), or sulfur dioxides (SOx) (Roy et al. 2014)

Fate and exposure

The recommended fate and exposure factors are based on Roy et al. (2012b) for average annual atmospheric fate factors and on Roy et al. (2012a) for estimating soil sensitivity, including pH changes. Roy et al. (2012b) applied the GEOS-Chem air quality model to translate emissions of NO_x, NHx, or SOx to fractions deposited on terrestrial systems. GEOS-Chem simulates the transport and deposition of multiple species simultaneously at a 2° × 2.5° resolution. Roy et al (2012a) developed sensitivity factors (SFs) that express the capacity of a soil system to buffer changes in deposition and respond to marginal changes in deposition. (These factors are mathematically equivalent to exposure factors, though an exposure factor often describes the fraction of the original contaminant available to cause an effect. In this section, we use the terminology and indicators adopted by Roy et al. (2012a), who refer to soil sensitivity as part of the fate calculation, rather than an exposure factor.) Among the soil indicators calculated is the soil solution pH, used in effect modelling. Spatially explicit soil sensitivity was modelled at the global scale with the PROFILE soil model, considering four soil chemical indicators to evaluate SFs for regional receiving environments.

Effect

The selected effect factor is based on Azevedo et al (2013b), which relates terrestrial acidification to changes in plant species diversity, estimating the potential losses of vascular plant species for different global biomes. To determine the effect on receiving ecosystems, the authors used empirical occurrence data of 2409 species and computed the species richness as the sum of present species at each 0.1 pH unit value within each biome finding considerable variability within them. The potentially not occurring fraction (PNOF) of species aggregated at the ecosystem (biome) level is valid for species communities, but not for single species.

3.5.4 General modelling considerations

Fate modelling

As all models are abstractions of physical systems of interest, the fate models recommended herein have limitations, as noted above. Advances in modelling may include higher spatial and temporal resolution, tracking more relevant species (inorganic and organic, dissolved and particulate forms), or improved physical and biogeochemical processes (e.g., for N and P, Beusen et al. 2015). In addition to considering general modelling improvements, we recommend that fate models consider background concentrations of species that may interact with the substance being modelled. This background modelling is accomplished with the GEOS-Chem model used for acidification (Roy et al. 2012b) but not for the other fate models.

Limiting nutrients

The recommended models for eutrophication model N and P separately, assuming that these nutrients limit growth of primary producers in marine and freshwater systems, respectively. Because N, P, and other nutrients may co-limit primary production (see section 3.2.2), we recommend that co-limitation be accounted for in future impact assessment models.

Effect modelling

In this and the preceding volume (Frischknecht and Jolliet 2016), the recommended LCIA damage endpoint is potentially disappeared fraction (PDF), which can be related to PAF (See Posthuma et al. [2002] for further discussion). At present, the PDF used in effect modelling in acidification and eutrophication refers to reversible, local impacts, as opposed to global.

Please see the cross-cutting issues chapter (Chapter 2) for further discussion on this distinction, which warrants more explicit treatment in LCIA models.

The underlying effect data recommended in this work (Azevedo et al. 2013b, 2013a) estimates effect factors for acidification and eutrophication from field observations of species presence or absence, reporting those values as PNOF. The marine effect model of Cosme et al. (2015) uses laboratory and field data to create a PAF estimate, PAF being a metric commonly applied to lab-based predictions. PNOF and PAF values can be directly interpreted as PDF, provided that the systems from which the predicted values were derived represent the systems for which the predicted damage is derived. Given the inclusion of field data in the effect derivations of both acidification and eutrophication, the task force assumes equivalency between PNOF, PAF, and PDF. Future modelling efforts should investigate this equivalency, but the task force recognizes that robust datasets for effect may be limited. We also recognize that empirical effect models may be limited by the quality and coverage of observational data, and that future LCIA modelling may also consider process-based models (e.g., Janssen et al. 2019).

We recommend consistency with previous guidance for LCIA developers to provide a set of characterisation factors for both the marginal and the average approach (Frischknecht et al. 2016; Frischknecht and Jolliet 2016). Figure 3 shows a notional PDF versus stressor curve, showing that species are lost at low stressor values (e.g., essential P is absent, or H+ values are low, leading to alkaline soils) and at high values, where toxic effects are present (eutrophication, or overly acidic soils cause aluminum mobilization). The marginal EF is calculated as the tangent at the current conditions. If data for the current situation of the considered stressor is not available, we recommend calculating the characterisation factor from the exposure-response curve at PDF 0.2. This point is recommended for consistency with the ecotoxicity approach, based on expert judgement in that group that 0.2 is more relevant for typical environmental exposure levels and does not incur the statistical uncertainty at lower values (such as 0.1) (Chapter 7).

Using the average approach requires defining a desired target (Figure 3). This could be a situation without human intervention, a political target, or the minimum of the exposure-response curve, which maximises species richness. As the desired target is not always available, we recommend creating average effect factors using the minimum of the species-response curve as the desired target (green "average" line in Figure 3.3). Often, the minimum is not captured in PDF or PAF data (e.g., Azevedo et al. [2013a, 2013a], as only the right-hand side (unshaded half in Figure 3.3) is modelled. In this case, we recommend taking the tangent at PDF=0.2 to determine the desired target.

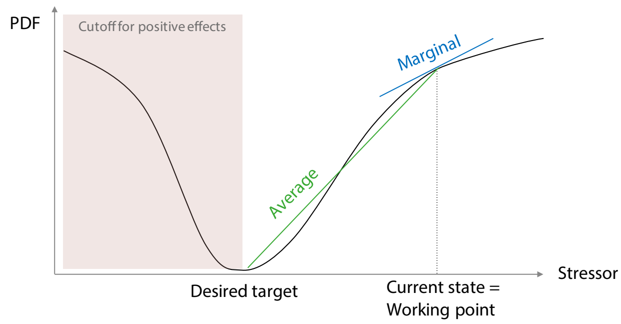

Figure 3.3. Conceptual species response to a stressor.

Positive impacts on species richness (the number of species in an ecosystem) are possible for both eutrophication and acidification, e.g., oligotrophic systems may have an increase in species diversity in a transformation to mesotrophic state, or species diversity may increase as acid inputs make a soil less alkaline. These may represent changes towards a system that is, however, more vulnerable, functionally distinct, or otherwise different than the target system. As discussed in Chapter 7 of this report, current LCIA modelling does not focus on the most sensitive species or weight the "value" of various species. Until approaches to adapt the PDF-stressor curve to reflect vulnerability, functional diversity, and other issues are developed, we recommend that EFs (and hence CFs) are set to zero when the current stressor level falls below the desired target, e.g., at low nutrient concentrations or high pH levels. This recommendation is in keeping with other LCIA categories, for which positive impacts are generally not considered. This recommendation also acknowledges the limitations of PDF as an indicator of pressure on ecosystems. To find the relationship of species to background concentrations in different locations a global database of current stressor levels is required; when such data are not available, we recommend that EFs be derived at the 0.2 PDF working point.

In order to provide the spatially-resolved characterisation factors noted above, spatially-resolved fate, exposure, and effect data must be available. At the time of writing, such effect data were available only for freshwater eutrophication. Therefore, the CFs for acidification and marine eutrophication that are presented in this work use the average EFs derived by their developers; i.e., these EFs are not reflective of current conditions.

Technosphere–ecosphere boundary

The eutrophication impacts considered rely on net emissions to a receiving body: P to river, N to river, and N to ocean. For the practitioner, it is unclear how to proceed if inventory represents applications to an agricultural field. While LC-Impact (Verones et al. 2016) and ReCiPe 2016 (Huijbregts et al. 2017, 2016) provide transfer fractions for P applications to soil, we recommend using a tiered approach for the estimate of net P and N emissions when life cycle inventory data is supplied as inputs to soil. It is recommended that practitioners adjust inventory data according to the goal and scope of their study, as outlined below.

- **Tier 1:** When agricultural systems are at the background level and fertilizer application data are provided, a default value of 10% can be applied to total P applied to agricultural soil to estimate P losses into freshwater (Bouwman et al. 2009). For nitrogen, IPCC (2006) provides a default factor to calculate nitrates leaching to surface water.
- **Tier 2:** When agricultural systems are at the foreground, recent guidelines developed by FAO (2018) provide methods to estimate P and N losses from feed production, storage, and livestock. This FAO work is the output of an international consensus effort and, as such, provides a consistent set of guidelines.
- **Tier 3:** When agricultural systems are at the foreground and detailed models (e.g., DAYCENT [Del Grosso et al. 2006], or Universal Soil Loss Equation [USLE] approaches [Scherer and Pfister 2015; Verones et al. 2016]) and data are available, such models are recommended to estimate N and P losses into the environment.

3.6 Characterisation factors (excerpt, including qualitative and quantitative discussion of variability and uncertainty)

Characterisation factors have been developed and provided in Excel and .csv files for native, country, and global scale resolutions. Based on the aggregation approach and effect factor approach described in sections 3.5 and 3.6, these CFs are based on many of the same underlying models as ReCiPe 2016, LC-Impact, and IMPACT World+. However, the CF developed in this work contain agricultural, non-agricultural, and general aggregation to country and world. At the endpoint level, for freshwater eutrophication only, linear and marginal effect factors based on current conditions are provided.

3.6.1 Biological oxygen demand and chemical oxygen demand

Although biological oxygen demand (BOD) and chemical oxygen demand (COD) contribute to eutrophication, most methods do not account for their contribution. For the short term, we suggest using the Redfield ratio, as is done in CML and IMPACT World+, which provide an equivalency factor of 0.022 kg phosphate-equivalents/1 kg BOD (or COD) (Bulle et al. 2019; Guinée et al. 2002). We strongly recommend the future development of CFs to model the actual environmental mechanism of eutrophication due to BOD and COD. This equivalency to phosphorus implies that BOD and COD impacts occur only in freshwater systems. This assumption is a simplification that relies on the Redfield-based connection between BOD and COD, P, and dissolved oxygen depletion in freshwater. In marine systems, this connection is more complex, given that DO depletion occurs in the benthic layers. Therefore, future LCIA methods should model the BOD-COD impact pathway explicitly.

3.6.2 Aggregation

In keeping with cross-cutting recommendations, we strongly recommend aggregating CFs/FFs from grid cells, to country, and finally global levels using different weighting factors to differentiate agricultural from non-agricultural uses. This acknowledges that N and P emission distributions vary strongly depending on the sector (agricultural areas vs. populated and industrialized areas). Practitioners may then apply the CFs relevant to the process studied (agricultural vs. non-agricultural activity). Such an approach has been demonstrated for water issues in the previous Pellston Workshop (Frischknecht and Jolliet 2016) and as a general framework (Bourgault 2013). Suggestions for aggregation data sources for the impact categories are the following:

Terrestrial acidification and freshwater eutrophication - Regarding agricultural emissions, FFs are weighted by N and P fertilizer application rates representative of 2013, gridded at a 0.5 degree resolution (Lu and Tian 2017). Regarding non-agricultural emissions, these FFs are weighted by population as a proxy for N-emitting industrial activities, P emitted in wastewater (the main source of P emissions beyond agriculture), or other emission sources.

Marine eutrophication - Regarding agricultural emissions, Cosme, Mayorga et al. (2017) FFs (at the river basin scale) are weighted by DIN emitted from agricultural soil estimated by the Global NEWS2 model at the same resolution (river basin) as the Cosme FF models. Regarding non-agricultural emissions, Cosme, Mayorga et al. (2017) FFs (at the river basin scale) are weighted by point source emissions estimated by the Global NEWS2 model at the same resolution (river basin).

3.6.3 Characterisation factors

The following sections present a summary of factors developed for the considered impact categories. Both midpoint and endpoint CFs are aggregated at country and global scale (Section 3.5). The eutrophication or acidification potential, at midpoint, and for native or aggregated (e.g., country) resolution can be normalised relative to the weighted, global factor according to the following:

$$CF\_normalised_{\text{grid i}} = CF_{\text{grid i}} / CF_{\text{global}}$$

Freshwater eutrophication

Table 3.1 summarises the range of values for freshwater eutrophication developed in this work, showing the differences between aggregation weights (agricultural, non-agricultural, and general). Only Average EF values have been used. The choice of aggregation can change the overall characterisation by up to two orders of magnitude, with strong 3 differences between non-agricultural and agricultural aggregation to country level.

Marine Eutrophication

Table 3.2 summarises the marine eutrophication values developed in this work, showing the differences between aggregation weights (agricultural, non-agricultural, and general). As with freshwater eutrophication, the introduction of different aggregation strategies results in variations up to two orders of magnitude.

The coupling of airborne fate factors with the recently developed marine eutrophication factors of Cosme results in a novel set of characterisation factors. These factors describe a variety of pathways that bring N emissions to the marine system, e.g., N emissions to air, deposition to soil, and transport to the marine environment. Future work to study the contributions of these pathways is warranted.

Terrestrial acidification

Table 3.3 summarises the terrestrial acidification values recommended in this work, showing the differences between aggregation weights (agricultural, non-agricultural, and general). For this impact category, the different aggregation strategies results in more modest variations, as the air transport mechanisms associated with deposition of acidifying substances are not tied to the hydrology of a region, as eutrophication mechanisms are.

3.7 Rice case study application

Impact scores for terrestrial acidification and freshwater eutrophication have been calculated for the three scenarios of the rice case study, which compare rice cultivation, processing, transport, and consumption in three sample locations: India, China, and Switzerland

Table 3.1. Summary statistics for country-level freshwater eutrophication factors. All factors are for P emissions to freshwater. Midpoint units are kg Peq, and endpoint are PDF.m3.yr.

Level	EF type	Substance	Emit	Via	Receive	Weight	10th percentile	50th percentile	90th percentile
Midpoint	None	P	Freshwater		Freshwater	Agric.	0.016	0.085	0.37
Midpoint	None	P	Freshwater		Freshwater	Non-Agric.	0.011	0.091	1.00
Midpoint	None	P	Freshwater		Freshwater	General	0.013	0.073	0.43
Endpoint	Average	P	Freshwater		Freshwater	Agric.	3.2E-3	0.019	0.22
Endpoint	Average	P	Freshwater		Freshwater	Non-Agric.	4.0E-3	0.029	0.51
Endpoint	Average	P	Freshwater		Freshwater	General	2.8E-3	0.016	0.24

Table 3.2. Summary statistics for country-level marine eutrophication factors. Midpoint units are kg Neq, and endpoint are PDF.m3.yr.

Level	EF type	Substance	Emit	Via	Receive	Weight	10th percentile	50th percentile	90th percentile
Midpoint	None	N	Freshwater		LME	Non-Agric.	0.023	0.84	2.2
Midpoint	None	N	Freshwater		LME	General	0.023	0.84	2.2
Midpoint	None	N	LME		LME	Non-Agric.	0.14	0.82	2.3
Midpoint	None	N	LME		LME	General	0.14	0.82	2.3
Midpoint	None	N	Soil		LME	Agric.	0.044	0.44	2.5
Midpoint	None	N	Soil		LME	General	0.044	0.44	2.5
Midpoint	None	NHx	Air	Freshwater	LME	Agric.	0.49	1.3	5.6
Midpoint	None	NHx	Air	Freshwater	LME	Non-Agric.	0.24	1.1	4.8
Midpoint	None	NHx	Air	Freshwater	LME	General	0.49	1.3	5.6
Midpoint	None	NHx	Air		LME	Agric.	0.21	1.6	16
Midpoint	None	NHx	Air		LME	Non-Agric.	0.13	1.5	13
Midpoint	None	NHx	Air		LME	General	0.22	1.5	16
Midpoint	None	NHx	Air	Soil	LME	Agric.	0.86	2.4	6.2
Midpoint	None	NHx	Air	Soil	LME	Non-Agric.	0.28	1.9	5.5
Midpoint	None	NHx	Air	Soil	LME	General	0.89	2.4	6.3
Midpoint	None	NOx	Air	Freshwater	LME	Agric.	0.25	0.85	4.7
Midpoint	None	NOx	Air	Freshwater	LME	Non-Agric.	0.15	0.58	3.7
Midpoint	None	NOx	Air	Freshwater	LME	General	0.26	0.85	4.5
Midpoint	None	NOx	Air		LME	Agric.	0.17	1.6	17
Midpoint	None	NOx	Air		LME	Non-Agric.	0.090	0.80	15
Midpoint	None	NOx	Air		LME	General	0.17	1.6	17
Midpoint	None	NOx	Air	Soil	LME	Agric.	0.59	1.8	6.6
Midpoint	None	NOx	Air	Soil	LME	Non-Agric.	0.35	1.5	5.9
Midpoint	None	NOx	Air	Soil	LME	General	0.61	1.8	6.6
Endpoint	Average	N	Freshwater		LME	Non-Agric.	6.3	258	1.2E+3
Endpoint	Average	N	Freshwater		LME	General	6.3	258	1.2E+3
Endpoint	Average	N	LME		LME	Non-Agric.	125	818	3.3E+3
Endpoint	Average	N	LME		LME	General	125	818	3.3E+3
Endpoint	Average	N	Soil		LME	Agric.	2.9	40	307
Endpoint	Average	N	Soil		LME	General	2.9	40	307
Endpoint	Average	NHx	Air	Freshwater	LME	Agric.	0.80	2.0	15
Endpoint	Average	NHx	Air	Freshwater	LME	Non-Agric.	0.34	1.8	13
Endpoint	Average	NHx	Air	Freshwater	LME	General	0.81	1.9	16
Endpoint	Average	NHx	Air		LME	Agric.	73	473	4.3E+3
Endpoint	Average	NHx	Air		LME	Non-Agric.	35	415	3.3E+3
Endpoint	Average	NHx	Air		LME	General	80	491	4.3E+3
Endpoint	Average	NHx	Air	Soil	LME	Agric.	16	40	158
Endpoint	Average	NHx	Air	Soil	LME	Non-Agric.	6.2	34	144
Endpoint	Average	NHx	Air	Soil	LME	General	16	41	153
Endpoint	Average	NOx	Air	Freshwater	LME	Agric.	0.19	0.67	6.6
Endpoint	Average	NOx	Air	Freshwater	LME	Non-Agric.	0.12	0.44	5.2
Endpoint	Average	NOx	Air	Freshwater	LME	General	0.19	0.67	6.7
Endpoint	Average	NOx	Air		LME	Agric.	17	163	1.8E+3
Endpoint	Average	NOx	Air		LME	Non-Agric.	10.0	91	1.5E+3
Endpoint	Average	NOx	Air		LME	General	18	163	1.9E+3
Endpoint	Average	NOx	Air	Soil	LME	Agric.	3.7	13	60
Endpoint	Average	NOx	Air	Soil	LME	Non-Agric.	2.3	9.7	49
Endpoint	Average	NOx	Air	Soil	LME	General	3.7	13	58

Table 3.3. Summary statistics for country-level terrestrial acidification factors. Midpoint units are kg SO2eq, and endpoint are PDF.m2.yr.

Level	EF type	Substance	Emit	Via	Receive	Weight	10th percentile	50th percentile	90th percentile
Midpoint	None	NHx	Air		Soil	Agric.	0.54	1.7	7.2
Midpoint	None	NHx	Air		Soil	Non-Agric.	0.20	1.2	5.7
Midpoint	None	NHx	Air		Soil	General	0.54	1.7	7.6
Midpoint	None	NOx	Air		Soil	Agric.	0.41	1.9	5.0
Midpoint	None	NOx	Air		Soil	Non-Agric.	0.25	1.2	4.5
Midpoint	None	NOx	Air		Soil	General	0.41	1.9	5.1
Midpoint	None	SOx	Air		Soil	Non-Agric.	0.21	1.1	4.1
Midpoint	None	SOx	Air		Soil	General	0.21	1.1	4.1
Endpoint	Average	NHx	Air		Soil	Agric.	6.6	21	53
Endpoint	Average	NHx	Air		Soil	Non-Agric.	2.6	16	49
Endpoint	Average	NHx	Air		Soil	General	6.8	21	53
Endpoint	Average	NOx	Air		Soil	Agric.	1.7	5.6	10
Endpoint	Average	NOx	Air		Soil	Non-Agric.	0.93	4.4	9.7
Endpoint	Average	NOx	Air		Soil	General	1.6	5.7	10
Endpoint	Average	SOx	Air		Soil	Non-Agric.	2.1	13	37

(consumed in Switzerland, but produced in the USA) (Frischknecht et al. 2016). This case study illustrates the importance of country-specific information with respect to acidification and eutrophication flows. With respect to inventory, the three systems have differences in emissions that are relevant for acidification and eutrophication, the focus of this analysis. The Swiss cooking scenario has substantially lower NH3 to air and P to freshwater, emitted by rice production sourced in the US, than the other two scenarios (Figure 3.4). The Chinese and Indian farm production process have identical emissions from ammonia and nitrogen oxides. The cooking method also influences inventory, as SO2 and NOx are emitted by the wood cooking stove in the Indian scenario.

The following figures show the relative importance of considering nitrogen inputs to marine systems. Although this task force recommends caution when applying endpoint values for marine eutrophication, this analysis illustrates the potential contribution from airborne emissions of nitrogen-containing substances (on a mass basis, these were evident in Figure 4). Figure 5 shows the variation in country-level characterisation factors relevant to this study (i.e., only CFs for flows in the study are shown). For the purposes of the case study, the CFs corresponding to a general aggregation were used. There is modest variation (up to a factor 5) among countries.

Figure 3.6 shows the endpoint characterisation of the three product systems, disaggregated with respect to elementary flow. In the Chinese and Indian cases, the contributions of NO_x and NH3 to marine eutrophication are some of the largest overall contributions to endpoint. The larger impact for India is due to the higher CF (Figure 3.5). In contrast to marine eutrophication, for all cases, the relatively small freshwater phosphorus contributions (most emissions are to soil) are driven by modest emissions coupled with relatively low characterisation factors.

3.8 Recommendations and outlook

3.8.1 Main recommendation - Short summarising theses

Characterisation factors

Freshwater eutrophication

Midpoint: Freshwater eutrophication potential, in Phosphorus-equivalents, based on Helmes et al. 2012: recommended.

Endpoint: P damage (PDF) to freshwater ecosystems based on Helmes et al. 2012 for fate and Azevedo et al. (2013a) for effect: recommended.

Marine eutrophication

Midpoint: Marine eutrophication potential in Nitrogen-equivalents, based on the fate modelling of Cosme, Mayorga et al. (2017): recommended.

Endpoint: N damages (PDF) on marine ecosystems,

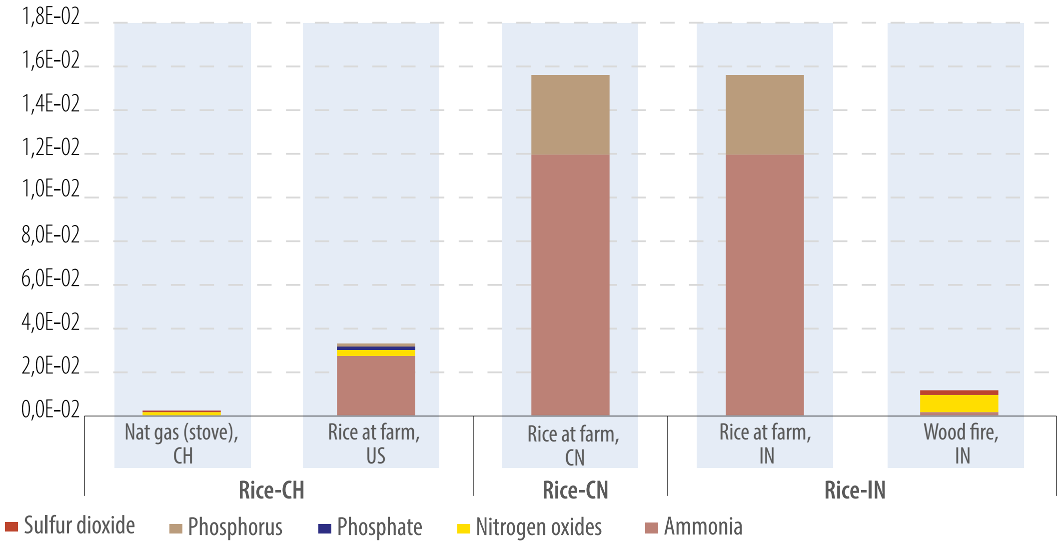

Figure 3.4. Inventory emissions for the rice case study, showing higher mass flows of NH3 and P in the China (CN) and India (IN) scenarios.

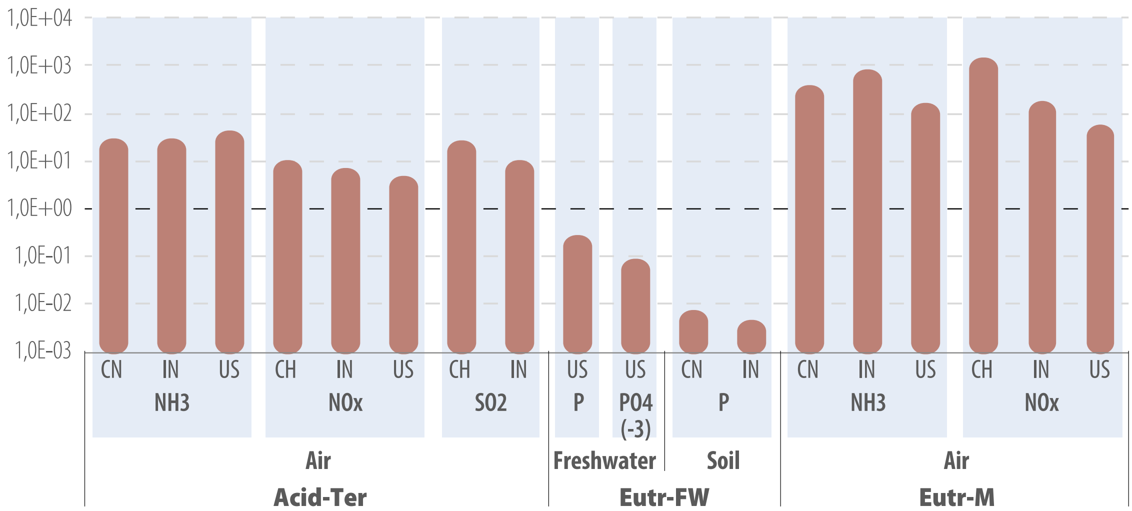

Figure 3.5. Comparison of CFs by location for inventory flows that are used in the case study.

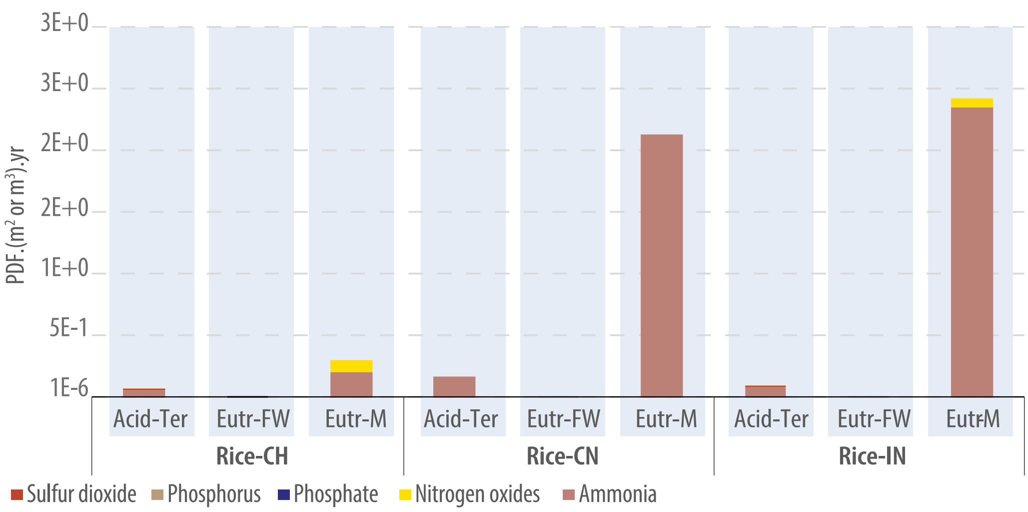

Figure 3.6. Characterisation of rice scenarios, showing higher impacts from NH3, NOx, and SO2 across scenarios, with modestly reduced impacts in the CN scenario.

based on Cosme and Hauschild (2017): suggested. Given the modelling uncertainties discussed in Section 3.5.2, the group highlights the limitations of the model and the importance of careful interpretation of results.

Terrestrial acidification

Midpoint: Terrestrial acidification potential in SO_2 -equivalents, based on Roy et al. (2012b): recommended.

Endpoint: PDF in terrestrial ecosystems, based on Azevedo et al. (2013): recommended.

Note: At endpoint level, the task force also makes a strong recommendation for further, location-specific case studies in which investigators with local knowledge of systems can evaluate the spatially explicit CFs in known circumstances, sharing their results in peer-reviewed publications.

Modelling approaches

We strongly recommend aggregating CFs and FFs from native scale (e.g., grid cells) to river basin (for freshwater eutrophication), country, and global levels using a weighting factor to differentiate agricultural from non-agricultural uses.

We strongly recommend using current environmental concentration as the working point on the effect curve, for both marginal and average effect factors. In the absence of these data, we recommend a working point of 0.2.

To determine the target state for average effect factors, we recommend using the point of minimum PDF. When this point is not available, we recommend taking the tangent at PDF=0.2 to determine the desired target (see Section 3.5.4 C).

We recommend that EFs (and hence CFs) are set to zero when the current environmental concentration falls below the desired target. This recommendation recognises the limitations of PDF as an indicator of ecological pressure; once approaches to capture vulnerability, functional diversity, etc. are developed, this recommendation should be revisited.

We suggest using an equivalency factor of 0.022 kg Phosphate/1 kg BOD (or COD) as an interim approach. We strongly recommend future development of CFs that reflect the actual environmental mechanism of BOD and COD.

We recommend further developing LCIA models to consider co-limitation, tracking impacts of both phosphorus and nitrogen in both freshwater and marine water bodies. At present, to maintain clarity in the recommendations and align with the current LCA practice, we consider nitrogen as the limiting nutrient in marine systems and phosphorus as the limiting nutrient in freshwater in these recommendations.

3.8.2 Judgment on quality, interim versus recommended status of the factors and recommendation

While the models presented here have undergone peer review and are published in various academic journals, the resulting CFs still need more case study applications to validate their functionality on a practical level and to identify further areas of improvement.

3.8.3 Applicability, maturity, and good practice for factors application

Interpretation

The recommended models for usage in LCIA have limitations, which were previously discussed. As a result, we recommend interpreting the LCA results in detail and communicating them correctly to avoid misunderstanding, as well as overestimations and underestimations. This includes the following aspects:

- Substances that are missing in the inventory and/or impact assessment. For example, in terrestrial eutrophication the only substances considered in the impact assessment are NOx, SO2, and NH3 because they are most relevant, although others might be critical as well. (See Section 1.2).
- If spatially explicit LCIA models are used, we recommend that the inventory cover the same spatial resolution to avoid the overestimation or underestimation of impacts. If this is not possible, we recommend it be stated clearly in the interpretation. This could also lead to a redefinition of the goal and scope. We suggest handling this as an iterative process.
- Measures of the uncertainty of model outputs are recommended to be estimated and communicated, per the guidance in the cross-cutting chapter (Chapter 2).
- Using PDF as an indicator to account for acidification and eutrophication leads to the possibility of having positive effects. Even though

we recommend that these positive effects are not considered at this stage (see Section 1.9.3) we recommend this possibility be communicated transparently, when applicable.

- The selected endpoint indicator is based on PDF. In general, and in particular for comparison to other models, we recommend the meaning of the indicator be communicated clearly (e.g., PAF may include effects other than death) and that LCIA model results using PDF, PNOF, or PAF be put into context, as these only represent the effect on measured species, and do not account for vulnerability, functional diversity, etc.

3.8.4 Link to inventory databases (needs for additional inventory features, needs for additional inventory flows, classification or differentiation etc.)

For LCAs of processes related to eutrophication or acidification, we recommend using regional inventory data when possible. If a practitioner uses site-generic data, an uncertainty analysis is recommended. This point denotes the importance of having the inventory databases correspond to the impact models available. In the case of agricultural activity, if inventory is supplied as an input (e.g., fertilizer or manure applied), rather than an emission, we recommend using the tiered approach described in Section 3.5.4D) to estimate emissions.

3.8.5 Roadmap for additional tests

While thorough validation of LCIA models is not feasible, spatially explicit fate and effect models can be evaluated against models from other domains, and LCIA models can be used in a regional application and tested against well-known local conditions. For example, acidification effects in Scandinavian regions, freshwater eutrophication in the US Great Lakes, or marine eutrophication in the Baltic Sea have been well-studied. Application of such case studies provides a level of ground-truthing that can provide valuable feedback regarding model performance. Ideally, model developers would track the use of their models in case studies, to gather feedback and improve the models. As a first step, our recommendations for characterisation models include encouragement to monitor performance in applications.

3.8.6 Next foreseen steps

The task force has implemented its recommendations in the CF files presented herein. However, the approaches presented here will be published in the peer-reviewed literature. The task force hopes that this guidance effort will spur further development for acidification and eutrophication modelling in LCIA.

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4. Human Toxicity

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4.1 Scope

Practitioners in life cycle assessment (LCA) consider human toxicity a major impact category that requires a set of characterisation factors for a large number of chemical substances. In this context, human toxicity refers to the disease burden attributable to exposure to chemical substances released throughout a product or service life cycle. However, there are significant challenges in developing quantitative human exposure and toxicity effect metrics for exposures to chemicals released into the environment, and for direct exposures to chemicals found in consumer products. Much of the available research and applications of health impact assessment of chemical stressors comes from the fields of toxicology and exposure science, where the focus is on data and methods designed for regulatory risk and safety assessments. Although this research provides an extensive repository of data and protocols for assessing human health impacts, current approaches for toxicology and risk assessment cannot be directly translated to calculate characterisation factors for use in comparative LCA studies. This is due to intrinsic differences in the boundary conditions and related assumptions of these frameworks. Information on comparing risk assessment and life cycle assessment with focus on human toxicity can be found elsewhere (e.g., Bare 2006).

Characterising human toxicity in the life cycle impact assessment (LCIA) phase of LCA has the goal of providing quantitative comparisons of the potential for chemicals to expose and harm human populations. LCIA focuses at the most likely range of exposure and harm for the median individual in a given human population. In contrast to LCIA, the goals of human health risk assessments are to provide one-sided confidence with regard to safety. Hence, such assessment is designed to ensure high confidence that an actual risk has not been underestimated—a practice that often relies on underlying "conservative" assumptions. In contrast, LCIA provides quantitative estimates of the capacity to cause harm and two-sided confidence intervals around these estimates. This is driven by the need for making substance and product-service system comparisons in LCA to identify best-in-class solutions. Using upper bound estimates of health effects could result in mis-classification in such comparisons and hence should be avoided.

Current practice for deriving LCIA human toxicity characterisation factors is incorporated in the global consensus model USEtox and its associated substance databases (Rosenbaum et al. 2008), focusing on inhalation and ingestion exposure, and related health effects from emissions to far-field compartments (air, water, soil) or a generic indoor compartment. However, despite reflecting as consensus model mature science (Hauschild et al. 2008), the current toxicity characterisation framework in LCIA has limitations that call for further improvement based on new scientific findings. The most essential improvements are related to:

1. Addressing spatiotemporal and population-level resolution to estimate impact potentials;
2. Addressing chemical substances in consumer products and in occupational settings, and adding related near-field human exposure pathways as defined in Fantke et al. (2016a), such as migration from material surfaces to human skin;
3. Extending the limited coverage in available substance toxicity dose-response data and models; and
4. Improving the coverage and quality of substance data.

These limitations motivated our efforts to provide additional guidance to help practitioners go beyond far-field and generic indoor emissions, and to take advantage of the latest research on near-field (i.e., vicinity of consumers or workers) exposure assessment (e.g., Jolliet et al. 2015; Fantke et al. 2016a), dose-response and severity models and data (e.g., Chiu and Slob 2015; Salomon et al. 2015; Forouzanfar et al. 2016).

During its scoping phase, the Human Toxicity Task Force enlisted leading experts from academia, business, government, and other sectors (e.g., non-profit and intergovernmental organisations) to develop a roadmap for advancing human toxicity characterisation in LCIA. The proposed roadmap included the discussion of a set of specific questions addressing: (1) approaches and data needed to determine human exposure and related toxicity effect indicators; (2) the validity and maturity of such approaches and data needed to represent human toxicity impacts for currently missing exposure pathways; and (3) the relevance and feasibility of considering essentiality and long-term emissions for metals. This last issue arises because of the persistence of metals and specific challenges associated with modelling human toxicity impacts for metal species.

The outcome of this scoping phase and related initial recommendations are detailed in Fantke et al. (2018). The findings and research priorities provided in these recommendations serve as the roadmap for the work described in the present chapter.

4.2 Impact pathway and review of approaches and indicators

Characterising human toxicity impacts must respect the boundary conditions of LCA to ensure the relevance and consistency of environmental impact comparisons among different products or services, life cycle stages, and other impact categories. We follow here the boundary conditions identified to be of importance to the characterisation of human health impacts in an LCIA context. Between 2003 and 2008, the Life Cycle Initiative provided initial guidance for characterising human toxicity impacts for substances emitted to the far-field (i.e., outdoor) environment (Hauschild et al. 2008; Westh et al. 2015). This effort was informed by model comparisons and expert elicitations (Jolliet et al. 2006; McKone et al. 2006), and resulted in the first version of the scientific consensus model USEtox (Rosenbaum et al. 2008; 2011), which was updated in 2015 with the introduction of a generic indoor air compartment (Rosenbaum et al. 2015).

The USEtox consensus-based modelling framework is considered a suitable starting point for characterising human toxicity impacts in LCIA (Fantke et al. 2018). In this framework, toxicity-related impacts on humans are described as a combination of human health effects h (aggregated into cancer and non-cancer effects, each having different severity), induced by exposure to chemicals, which distribute among the various environmental far-field compartments c (e.g., outdoor air, water, and soil) and reach humans via exposure pathways x (e.g., inhalation of air, ingestion of food). These factors are combined for each emission E in a matrix $\mathbf{CF}_E \in \mathbb{R}^{h \times c}$ of characterisation factors expressed as disability-adjusted life years (DALY) per kg emitted [DALY/kg$_{\text{emitted}}$], relating impacts on humans via health effects h to unit emissions into environmental compartments c per functional unit:

$$\mathbf{CF}_E = \overbrace{\mathbf{SF}\,\mathbf{DRF}}^{\mathbf{EF}}\ \overbrace{\mathbf{XF}\,\mathbf{FF}}^{\mathbf{iF}} = \mathbf{EF}\,\mathbf{iF} \qquad (1)$$

where diagonal matrix $\mathbf{SF} \in \mathbb{R}^{h \times h}$ of severity factors [DALY/case] for health effects h, multiplies matrix $\mathbf{DRF} \in \mathbb{R}^{h \times e}$ of dose-response slope factors [cases/kg$_{\text{intake}}$] for health effects h, via exposure pathways x Matrices $\mathbf{SF}$ and $\mathbf{DRF}$ are conveniently combined into a matrix $\mathbf{EF}$ of human toxicity effect factors [DALY/kg$_{\text{intake}}$]. This matrix multiplies matrix $\mathbf{iF} \in \mathbb{R}^{x \times c} = \mathbf{XF}\,\mathbf{FF}$ of human intake fractions [kg$_{\text{intake}}$/kg$_{\text{emitted}}$], which is obtained as from the product of matrix $\mathbf{XF} \in \mathbb{R}^{x \times c}$ of human exposure factors [kg$_{\text{intake}}$/d per kg$_{\text{in compartment}}$] from receiving environmental compartments c via exposure pathways x and square matrix $\mathbf{FF} \in \mathbb{R}^{c \times c}$ of environmental fate factors [kg$_{\text{in compartment}}$ per kg$_{\text{emitted}}$/d] from emission to receiving compartments c.

In order to characterise fate processes and human exposure pathways in the near-field (consumer and occupational) environments, and consistently combine these with existing far-field (outdoor environment) processes and pathways, we reviewed a number of available exposure-model options that can be used to address chemical substances in consumer products (Huang et al. 2017). We used this review to make recommendations on an approach that considers human exposures during and after product use, exposure of bystanders (i.e., humans exposed by being located close to e.g., agricultural emission sources), and occupational exposure pathways. We recommend the use of consistent mass-balance models to link near-field exposures to human receptors, following the recommendations of Fantke et al. (2016a), who discuss the applicability of such mass-balance approach for human toxicity characterisation in LCIA. This approach combines near-field (i.e., household environments for consumers and occupational environments for workers) with far-field (i.e., outdoor environments) exposures into a metric that incorporates the interactions of humans with both types of environments via dermal, mouthing, inhalation, and oral exposure pathways and potential feedback via for example exhalation. We identified the product intake fraction (PiF) proposed by Jolliet et al. (2015) as a useful metric linking human intake via all exposure routes directly to the substance mass in products (instead of linking human intake to environmental emissions). In contrast to the approach using iF, which is based on inverting a matrix of rate constants (yielding matrix $\mathbf{FF}$), we propose to use a matrix $\mathbf{PiF} \in \mathbb{R}^{x \times c}$ of product intake fractions, which includes as subset all intake fractions of matrix $\mathbf{iF}$ but additionally includes direct exposure to chemicals in any product, based on the combination of mass transfer fractions between all compartments (not shown here, but described in detail in Fantke et al. (2016a). Using PiF, we get an extended matrix $\mathbf{CF}_P \in \mathbb{R}^{h \times c}$ of characterisation factors per kg in product application P [DALY/kg$_{\text{in product}}$], relating impacts on humans via health effects h to the unit mass of a chemical in a product application compartment c per functional unit:

$$\mathbf{CF}_P = \mathbf{SF\ DRF\ PiF} \quad (2)$$

Figure 4.1 illustrates how, in contrast to the receptor-oriented perspective followed in risk- and safety-oriented assessments, the PiF-based framework primarily takes an emitter or product-oriented perspective (Fantke and Ernstoff 2018). This product-oriented approach is focused on providing a basis for comparisons of life cycle-based toxicity impacts rather than on assuring safety. In order to compare across substances, it is important to account for uncertainties that can vary among substances as a function of differences in substance-specific physicochemical properties and exposure potentials.

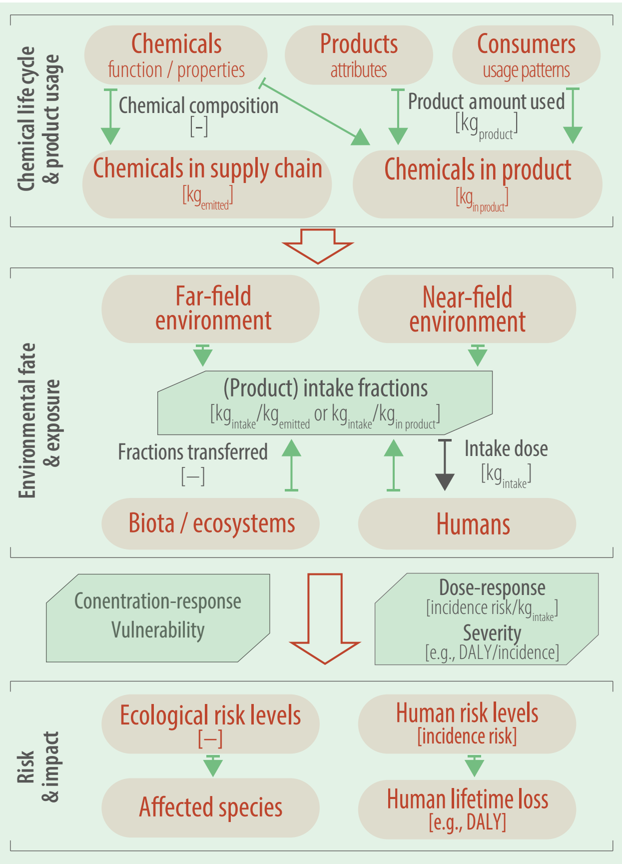

Figure 4.1. An illustration of the extended near-field and far-field framework for assessing combined human exposure from a full product-service system (adapted from Fantke et al. 2016a; UN Environment 2019). While the present chapter focuses on human impacts, certain fractions of chemicals in products can also reach the environment and affect ecological receptors. The related impact pathways are covered in Chapter 7.

4.3 Process and criteria applied and process to select the indicator(s)

In support of developing a combined near-field and far-field exposure assessment framework that is compatible with the existing LCIA approach for human toxicity characterisation, relevant fate and exposure mechanisms were identified as a first step. A wide range of existing approaches to address near-field fate and exposure transfers and processes have been recently evaluated (Huang et al. 2017; Shin et al. 2017). Both reviews point out the lack of and need for integration of various pathways within existing cumulative exposure models. They demonstrated the importance of a model framework that not only tracks exposure during product use but also the range of other potentially important exposure pathways. This includes exposure after product use, exposure due to indoor air releases, exposure due to subsequent outdoor air releases, and exposure from volatilization and surface water discharges at waste-water treatment plants. We use these findings as a starting point to identify fate and exposure mechanisms that need to be considered in LCIA and to screen existing models for their suitability to be used in a comparative, mass balance-based framework.

As a follow-up to the initial scoping phase, we organised three workshops to discuss the proposed scoping questions and make initial recommendations for action. These workshops provided the essential foundation and supporting information for the work carried out by the Human Toxicity Task Force. The first workshop was held at the International Society of Exposure Science (ISES) annual meeting in Utrecht, Netherlands, in October 2016, with 40 exposure and toxicity experts attending from nine countries, who identified and discussed the main scientific questions and challenges. A subsequent workshop was organized at the Society of Environmental Toxicology and Chemistry (SETAC) annual meeting in Brussels in May 2017. Here, nine researchers associated with the USEtox International Centre and 15 experts and representatives from different metal industry associations focused on evaluating recent models and data relating to human toxicity characterisation of metals and the set of findings from Eurometaux meeting in 2014 (Eurometaux 2014). A final workshop was organised at the ISES annual meeting in Research Triangle Park, North Carolina, in October 2017, where 20 toxicity and exposure science experts from industry, government agencies, and academia discussed approaches and data needed to establish improved dose-response and disease severity factors for a large number of substances. Findings of these three scoping workshops are discussed in Fantke et al. (2018), constituting the background for the indicators, models, and data presented in the following sections.

4.3.1 Data transparency

The principles and overarching aims of LCIA state that analyses should aim for transparency, such that data used are generally available and uses of such data are documented in a way that analyses could be repeated by others (Hertwich et al. 2018). Therefore, LCIA human toxicity method developers and LCA practitioners alike should strive to use existing public data sources and explain how the data used have been extracted from specific sources. Since many public sources are updated or otherwise modified over time, the time at which data used were taken should be documented ideally along with including a version number (Hauschild et al. 2018).

4.3.2 Data confidentiality issues

Often, there are few or even no publicly available exposure (e.g., product use patterns or chemical ingredient quantities in products) or toxicity (e.g., human dose-response information) data. To omit chemicals without data from the analysis biases LCA results and can mislead related decisions, so assiduous efforts need to be made to obtain essential data for all substances that are relevant in an LCA context. There may be sources of data on potential toxicity of products based on chemical formulation or data on other aspects of product composition and use that are proprietary or otherwise not publicly available. For example, toxicity data that have been submitted under the European REACH regulation (European Commission 2006) are available publicly only in highly summarised form, or companies may develop proprietary toxicity data. Such data may be obtained for limited uses in a form useful to the conduct of an LCIA, with legal restrictions on permitted uses or disclosure, presenting a challenge to the conduct of a fully transparent analysis. It may be possible, however, to name the source of the data (though not reveal the data themselves), or to release some level of aggregation of the data. In such cases, it is important to provide the fullest allowable information about how the data were originally obtained, how the permission to use these data was granted, and as much detail about the nature of the unreleased data as is possible to provide.

Some data are needed for a single analysis, while some data might be usefully embedded in analyses for future use, or in software implementations or tools that are themselves to be made publicly available. In such cases, it will be necessary to ensure that using these data is permitted, and steps will likely need to be taken to ensure that the data cannot be extracted (or inferred by "reverse engineering") by users of the products containing the embedded data in hidden form. Similarly, comparison of different scenarios may entail proprietary inputs for one scenario that cannot be legally shared. Those inputs may need to be combined with or otherwise interact with other components within the analytical process, and the partial or intermediate results of these interactions may be necessary to preserve for the full analysis, yet they may allow inference about the proprietary inputs (by reversing calculations that use both public and private information). In such a case, care will need to be taken that the intermediate results themselves are not publicly available, or that they are sufficiently kept confidential in any wider distribution of the analysis. We strongly recommend that all of these compromises with the ideal of full availability of exposure and toxicity data are considered only when necessary, to improve on the still less desirable use of surrogate methods for undertaking analyses that could have been done with directly relevant data.

4.4 Description of indicator(s) selected

4.4.1 Human exposure factors

Assessing human exposure to chemicals in LCIA historically builds on the chemical mass emitted to the far-field environment (e.g., air, water, soil) quantified over the entire life cycle of products or services per functional unit (FU), which is the common basis of comparing the environmental performance of products or services (e.g., for a body lotion, the FU may be to increase skin hydration of 1 square meter of skin by 30% during 4 hours). The emitted chemical mass is then characterised in terms of its human exposure using multimedia mass balance models simulating environmental fate processes (e.g., inter-compartment transfers, such as between air and soil, as well as within-compartment degradations) and human exposure pathways (e.g., inhalation of air and ingestion of drinking water and food) (McKone and Enoch 2002; Pennington et al. 2005; Rosenbaum et al. 2008; van Zelm et al. 2009).

Multimedia fate and human exposure are typically assessed in LCIA using the human intake fraction (iF) relating population intake to mass emitted (Bennett et al. 2002). For assessing near-field exposure to chemicals in consumer products, the product intake fraction (PiF) was recently introduced in analogy to and compatible with iF (Jolliet et al. 2015; Ernstoff et al. 2016; Fantke et al. 2016a). Despite their relevance to potentially dominate overall exposure to chemicals (Wambaugh et al. 2014; Shin et al. 2015; Csiszar et al. 2016), near-field exposure pathways are currently not considered in operational LCIA models, except for the pathway of inhaling chemicals emitted to a generic indoor air compartment, which has recently been incorporated into USEtox (Rosenbaum et al. 2015). When combining near-field and far-field environments for human exposure, not only exposure of the general population (including consumers or product users and workers) to chemicals in outdoor environments (focus in existing LCIA toxicity characterisation models), but also direct exposures of consumers during product use and exposures in occupational environments can be considered. In certain decision contexts, it might be relevant to then report results for product use-related exposure of consumers separately from results for emission-related exposures of the general population and workers, because non-users of a product do no usually receive benefits from the functional unit for which the LCA is performed.

Building on these developments, we recommend developing a framework that considers both far-field and near-field environments in a consistent way to account for all relevant multimedia fate processes (i.e., transfers within and between near-field and far-field environments) and exposure pathways. As a starting point, we recommend building on the existing USEtox consensus model for far-field environmental fate and exposure (Rosenbaum et al. 2008) by adding near-field exposure compartments so as to maintain mass balance by following the conceptual framework proposed by Fantke et al. (2016a).

To operationalise such a framework in LCIA for assessing chemicals occurring in the various consumer product types (e.g., building materials, food contact materials, and cosmetics), different sets of near-field transfer and fate processes need to be considered. Based on these considerations, a suite of underlying models needs to be designed that are consistently integrated in the overall modelling framework. More specifically, all underlying, product type specific models need to follow mass balance principles, need to be applicable for calculating exposure to hundreds or thousands of chemicals in consumer products in LCIA, and need to address the relevant fate and exposure mechanisms (Fantke et al. 2016a).

4.4.2 Human toxicity effect factors

Human toxicity indicators are ideally derived directly from information on chemical potency in humans where available. However, for most chemicals, human toxicity data are not available. Thus, indicators of human toxicity are usually derived from animal experiments or, when such data are missing, from quantitative structure-activity relationships (QSAR) or other sources (Jolliet and Fantke 2015). These toxicity measures are extrapolated from animals to humans, and consideration of human variability in sensitivity is usually incorporated. Based on these toxicity assessments, an effect slope factor is derived, representing a change in human population response per unit change of exposure. These indicators can be derived both for carcinogenic and non-carcinogenic toxicity endpoints, depending on the chemical-specific data available. However, most animal toxicity assessment results are specific for cancer endpoints, while being much less specific for non-cancer endpoints. In order to allow for considering the various health endpoints obtained from (human and animal) toxicity test studies, the general approach in LCIA toxicity characterisation is to aggregate them into cancer and non-cancer effects.

The human toxicity effect factor is combined with exposure and effect severity factors to derive the human toxicity characterisation factor. Severity factors translate an estimated human response to units of disability-adjusted life years (DALYs). Average severity factors for non-cancer and cancer outcomes have earlier been derived based on incidence-weighted DALYs from the Global Burden of Disease (GBD) research (Huijbregts et al. 2005). Based on latest work in dose-response modelling (WHO 2014; Chiu and Slob 2015; Chiu et al. 2018) and GBD (Salomon et al. 2015; Forouzanfar et al. 2016) studies, we recommend refining the approaches for the selection of toxicity data, extrapolation of these data to derive effect factors for non-cancer endpoints, and the estimation of severity factors associated with non-cancer responses.

4.5 Model, method, and specific issues addressed

4.5.1 Human exposure models and data sources

In order to develop a portfolio of product archetypes, we consulted US EPA stochastic human exposure and dose simulation (SHEDS) consumer product categories (Isaacs et al. 2014) and the European ConsExpo program (Delmaar et al. 2005). We then selected based on the above-described literature review (Huang et al. 2017) five main models that we included in our framework for assessing various near-field exposure scenarios, namely 'direct near-field emission,' 'article interior,' 'skin surface layer,' 'object surface,' and 'food contact material' covering a variety of exposure pathways. Table 4.1 summarises the direct chemical transfer fractions that are determined by each model and the respective exposure pathways. These models have been incorporated into the matrix framework described in Fantke et al. (2016a) to address consumer exposure. Direct emissions to the near-field (i.e., indoor) environment are consistently coupled with far-field compartments. Extending the matrix framework presented in Equation 1 by these near-field environments and pathways now provides an approach for consistently estimating exposures and related impacts for product users as well as non-users and the general population in Equation 2. As a next step, it would also be important to consider exposures in the occupational environment to worker populations (Kijko et al. 2016). Thus, it is important to maintain the flexibility of the matrix framework so that additional or alternative exposure models or modules can be incorporated and implemented.

4.5.2 Human Toxicity Models and Data Sources

The human dose-response approach used to derive the human toxicity dose-response factor (DRF) in current LCIA models, such as USEtox, is based on recommendations of an expert workshop held within the UNEP-SETAC Life Cycle Initiative in 2004 as part of a scientific consensus-building process (McKone et al. 2006). This approach expresses human toxicity potential as a combination of the ratios of intake fractions to doses inducing a 50% effect response over background (ED50s) for non-cancer endpoints, and to median tumour doses (TD50s) for cancer health endpoints, keeping inhalation and ingestion exposure routes separate and differentiating between the contributions of cancer and non-cancer effects. As explained in McKone et al. (2006), the choice of 50% response level metrics rather than no-effect metrics or reference doses, provides a more robust comparison of toxicity. However, several potential limitations have been identified with this approach:

1. The assumption of zero effect for chemicals that

Table 4.1. Selected underlying near-field exposure models with main direct transfer fractions, exposure pathways, example products covered, and key references.

Model	Main transfers and compartments considered	Direct exposure pathways	Product example	Key references
Direct near-field emission	Emissions to near-person, indoor, urban or continental air, to surface water, agricultural and natural1 soil, WWTP[2] and STP[3]	Inhalation and gaseous dermal uptake, ingestion pathways associated with the indoor environment	All chemical emissions to indoor environmental compartments	Rosenbaum et al. (2008; 2015)
Article interior	Transfers from chemicals in article interior to near-person air or indoor air, also accounting for the long-term absorption on the walls for SVOCs[4]	Dermal contact with article surface, dust ingestion in addition to inhalation and gaseous dermal uptake	Chemicals encapsulated in article interior, building materials, articles, toys, or arts and crafts	Huang and Jolliet (2016)
Skin surface layer	Transfer from skin surface layer to near-person air, to human epidermis, and to WWTP[2]	Direct dermal aqueous uptake in addition to inhalation and gaseous dermal uptake	Personal care products, hand dishwashing	Csiszar et al. (2016)
Object surface	Transfer from object surface to near-person air, and indoor air	Dermal contact	Surface cleaner detergents	Ernstoff et al. (2016)
Food contact material	Transfer from food packaging to food	Dermal contact, food ingestion	Food packaging	Ernstoff et al. (2017)

[1]Natural soil is on areas outside of managed agricultural and forest lands, [2]Wastewater treatment plant, [3]Solid waste treatment plant (currently referring to landfills, but models can be added for e.g., waste incineration), [4]Semi-volatile organic compounds.

lack definitive hazard assessments or conventional dose-response data;

2. The lack of quantification of uncertainty and variability in the predicted dose-response relationships;
3. The assumption of linearity from ED50s to zero exposure, particularly for non-cancer endpoints for which non-linear dose-response relationships are generally expected; and
4. The lack of accounting for non-monotonic dose-response curves, such as those for essential metals, where incremental exposures may be either beneficial or detrimental, depending on the nutritional status of the exposed individuals.

We implemented a number of recent scientific advances in dose-response assessment of human toxicity in order to address these issues, focusing on non-cancer effects, for which there have been the most significant advances in methodology, application of new methods, and data availability in recent years. Additional work is required to implement recent scientific advances for cancer endpoints, such as deriving new points of departure (PODs) from reanalysis of tumour bioassay data. The POD is the point on a toxicological dose-response curve where an effect or no effect level can be established from experimental data, marking the starting point for further extrapolation to a desired dose. We suggest this be considered in the future in order to harmonise with the proposed updates for non-cancer effects. Until such advances are available, it is recommended to follow the existing approach for cancer effects (Crettaz et al. 2002) using TD50 data from the Carcinogenic Potency Database (CPDB) (Gold et al. 2011).

For issue (1), we have developed an updated hierarchy of data sources to identify an appropriate POD from which DRFs can be derived, as shown in Figure 4.2 (left panel), resulting in applicability to a much wider range of chemicals than is currently considered in LCIA. These sources include a newly available US EPA database of experimental *in vivo* animal toxicity data (see Table 4.2), a recently published QSAR model for predicting regulatory toxicity values (Wignall et al. 2018), and, as a fall-back solution, adaption of the threshold of toxicological concern (TTC) concept to specify a "conservative" no-observable adverse effect level (NOAEL) (Kroes et al. 2005) by applying a safety factor to the TTC. Regulatory values or experimental animal data (e.g., Table 4.2) are preferred, and if these are not available, estimation methods can be applied. Currently, we consider QSARs to have a wider applicability domain and to be more "fit for purpose" in predicting *in vivo* PODs in comparison with other new approach methods (NAMs), such as the use of *in vitro* high throughput screening (HTS) data and *in vitro* to *in vivo* extrapolation (IVIVE) methods (Wetmore et al. 2015; Wignall et al. 2018). Nonetheless, as NAMs continue to advance, the hierarchy can be augmented to incorporate such approaches as appropriate. On the other end of the spectrum, although human epidemiological data are in principle preferred over other types of hazard data, the vast majority of such studies lack the quantitative exposure data necessary to quantify dose-response relationships. Advances in exposure assessment approaches used in environmental epidemiology, such as the use of biomonitoring, may enable broader use of such data in the future, though this is likely to be reflected in "definitive" health assessments that are already at the top of the hierarchy.

For issues (2) and (3), we have adapted recent work by the World Health Organization's International Programme on Chemical Safety (WHO/IPCS) that developed a comprehensive framework to extend the usual risk assessment approaches to more formally incorporate non-linear dose-response relationships, uncertainty, and variability (WHO 2014; Chiu and Slob 2015; Chiu et al. 2018). As illustrated in Figure 4.2 (right panel), this approach first incorporates uncertainty in the POD; then implements a number of POD-specific probabilistic extrapolations to derive a human $ED50_H$; and finally predicts a human effect dose inducing a 10% response over background in humans ($ED10_H$) based on combining a non-linear log-normal model for human variability and a data-derived uncertainty distribution for the extent of human variability (i.e., variance of log-normal distribution). The DRF is then derived by making a linear extrapolation from the human $ED10_H$, with both the median and 90% confidence interval (CI) reported.

At first glance, it may appear that the only change from the approach recommended in 2004 is the use of the $ED10_H$ instead of the $ED50_H$ for linear extrapolation. However, our new approach has several important improvements. For instance, due to more comprehensive database coverage, this approach is applicable to many more chemicals than before (addressing Issue [1], above). Additionally, the new approach propagates uncertainty throughout the entire process, leading to more robust predictions as well as a quantitative characterisation of uncertainty, as recommended in and addressing Issue (2) above. It also addresses both dichotomous (yes/no response, where the response is either proportional to the dose = deterministic dichotomous, e.g., alcohol intoxication; or where the probability of response is proportional to the dose = stochastic dichotomous, e.g., cancer) and continuous (variable response, e.g., weight loss) dose-response types, which were not explicitly differentiated in the earlier approaches. Finally, the choice of $ED10_H$ is justified by multiple lines of reasoning related to the non-linearity of the underlying dose-response relationship:

- First, the $ED10_H$ is likely to be closer to the range of actual human exposures than the $ED50_H$, as well as being more consistent with the idea of additivity to background responses due to cumulative exposures and pre-existing risk factors (Zeise et al. 2013). Thus, using the $ED10_H$ is likely to more accurately reflect actual dose-response relationships.
- Second, it is recognised that a non-linear dose-response relationship continuously changes with changing exposure, so that given perfect information, the effect of a small incremental exposure evaluated in LCIA would be derived from the marginal slope at the current ("working point") exposure. However, based on analyses across a large number of compounds the uncertainty in dose-response relationships begins to diverge below a 1% response, being highly sensitive to the assumed shapes of both the uncertainty and variability distributions (Crump et al. 2010; Chiu et al. 2018).
- Finally, in analyses across a large number of compounds, the central tendency linearly extrapolated slope from $ED10_H$ is approximately equal to that of the marginal slope at $ED1_H$ (own analysis).

Together, these observations suggest that the linearly extrapolated slope from $ED10_H$ represents a *reasonable* estimate for the incremental effect of incremental exposures throughout the range likely to be relevant for application in LCIA.

With respect to issue (4), it is recognised that in many human populations, a significant fraction of the population may be deficient for essential metals (Lim et al. 2012; Forouzanfar et al. 2016; Gakidou et al. 2017). Thus, these individuals would not be "at risk" for human toxicity effects with any incremental exposure to these substances given current background levels (Milton et al. 2017). To address this issue, we propose that the DRF be multiplied only by the fraction of the population who already has adequate intake.

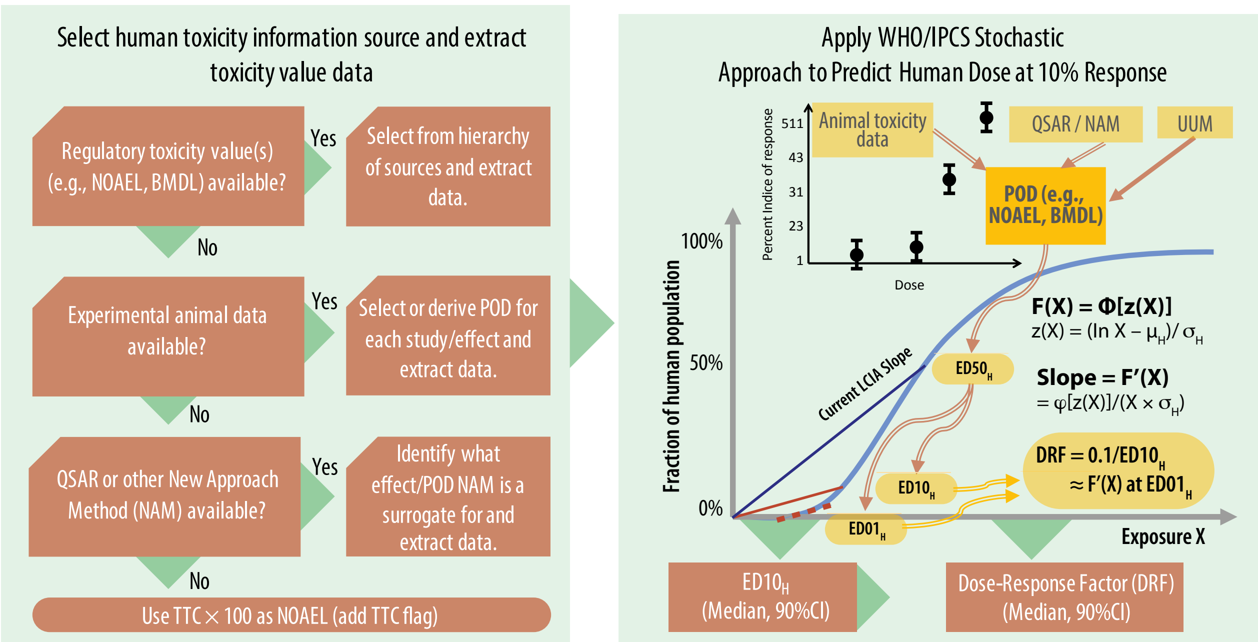

Figure 4.2. Overview of the new approach to Dose-Response Factor (DRF) determination. Left panel: Process for identifying point of departure (POD) data suitable for DRF derivation (e.g., NOAEL or BMDL). Right panel: Summary of the approach to derive the DRF from available POD data. Within the inset, each of the red-white arrows indicates a step where uncertainty is incorporated or propagated probabilistically.

Thereby, only the fraction of the population at risk is considered, e.g., the fraction of the population above the bioequivalent high limit corresponding to the Tolerable Upper Intake Level for the considered nutrient. Possible benefit from increased exposure to the portion of the population that is nutritionally deficient can be modelled separately.

Table 4.2. Number of available *in vivo* animal studies in the National Center for Computational Toxicology (NCCT) Toxicity Value Database (comptox.epa.gov/dashboard) by outcome study type and exposure route.

Outcome study type	Exposure route		
	Oral	Inhalation	Dermal
All acute	16350		
All repeat dose	5036		
Acute	16167	938	396
Subacute/short-term	581	10	25
Subchronic	1559	100	51
Repeat dose	343	131	63
Chronic	3355	648	22
Cancer	629	349	71
Developmental*	959	86	29
Reproductive*	719	49	10
Reproductive/developmental*	33		

*For a discussion of these outcome types see Section 4.5.3 on severity factors.

4.5.3 Severity factors

Integration of the dose-response curve approaches described in Section 4.5.2 provides an estimate of the population response at a given incremental chemical exposure level. However, the assessment of damage of the exposure on human health, which is commonly estimated in terms of lifetime loss, requires estimation not only of the population response, but also requires assignment of severity to the predicted responses in order to estimate the DALY associated with the incremental exposure. Huijbregts et al. (2005) provided estimates of incidence-weighted average DALY associated with a range of both cancer and non-cancer health endpoints of significance to the global human disease burden. They proposed that impacts could be assessed using these average DALY values, albeit with high uncertainty, particularly for the non-cancer endpoints, even though responses estimated from animal toxicity data can rarely be mapped to specific human diseases.

We propose that the previous approach is refined to address at least one additional subset of non-cancer responses separately from the other non-cancer responses. Substances that cause birth defects may be of special interest because of the clear dichotomous nature of the response, the presence of directly analogous disease states in humans, as well as because of the severity and duration of the outcome (US EPA 1991). Huijbregts et al. (2005) included a group of disease categories designated in the Global Burden of Disease (GBD) databases as congenital anomalies (birth defects) in the calculation of "average" DALY values for non-cancer outcomes. However, inclusion of these endpoints in the broader non-cancer category potentially severely under-weights such outcomes. Separation of this category of effects seems potentially justifiable from both a mechanistic and from a statistical point of view, given the heterogeneity in DALY between this category and other categories (Hay et al. 2017). The term "congenital anomalies" as used in the GBD and in public health has medical origins and refers in the context of toxicity data to "reproductive/developmental toxicity" effects. There is a spectrum of effect outcomes that falls into the category of reproductive/developmental toxicity. Developmental outcomes are effects that manifest in the offspring, while reproductive effects are those that affect the fertility or function of a parent for reproduction. This entire category of reproductive/developmental toxicity is a category that draws special attention in the regulatory world (along with cancer and mutagenesis), for example, shown in the "CMR" (carcinogenicity, mutagenicity, reproductive/developmental toxicity) designation [European Commission 2008]). Developmental outcomes thereby range in their severity from mild to extreme. However, the key for all reproductive or developmental effects is that they have the potential to adversely affect human organisms for their entire lifetime, either because they were never born (effects on reproduction) or because they were born with either functional or morphological deficits (effects on development).

Table 4.3 presents incidence-weighted DALY values for all non-cancer endpoints from Huijbregts et al. (2005), as well as separate values for the reproductive or developmental effects and other non-cancer diseases. Separation of the reproductive/developmental category from the other non-cancer responses results in a substantial decrease in the uncertainty associated with the average non-cancer (other than reproductive or developmental effects) DALY values. The reproductive/

developmental DALY should be applied for any substance for which the effect factor is derived from reproductive or developmental outcomes. In addition to this separation, we recommend that DALY values per incidence for both categories be updated with the most recent GBD statistics (Salomon et al. 2015).

Table 4.3. Incidence-weighted DALY/incidence values for all non-cancer endpoints, reproductive/developmental endpoints, and all other non-cancer effects, based on data from Huijbregts et al. (2005).

Disease category	DALY/ incidence [year]	Estimated uncertainty factor [-][a]
Cancer	11.5	2.8
Reproductive/ developmental[b], average	44.1	11
Other non-cancer, average	2.4	6.5

[a]Unitless, square root of the ratio of the weighted p97.5 to p2.5 of the contributing condition DALYs. Value from Huijbregts et al. (2005) for all non-cancer endpoints; value calculated from subsets as presented in Table 2 of that publication.
[b]Denoted in Huijbregts et al. (2005) as "congenital anomalies"

4.5.4 Applicability domain

The applicability domain of the models developed for this effort must be considered. Fate and exposure models are well developed for neutral organic chemicals with log Kow >1 and <8, and are routinely used within regulatory instruments for estimating environmental concentrations and human exposure (Cowan et al. 1995; Mackay 2001; European Commission 2003). However, it has been demonstrated that a considerable fraction of ionisable organic chemicals are used in commerce fall outside the applicability domain of several existing tools (Buser et al. 2012). Additionally, there are a number of other chemical classes, such as multi-constituent substances (i.e., substances consisting of two or more main chemical constituents as compared to mixtures, which are intentionally formulated using several chemicals), unknown or variable composition materials, complex reaction products or biological matrices, polymers, and surfactants, which also fall outside the applicability domain of models used in LCIA. Consistent with the recommendations of good modelling practice (e.g., Buser et al. 2012; EFSA 2014), it is strongly recommended that models provide the appropriate transparency with respect to applicability domain for users, and flag instances when a chemical to be assessed falls outside the domain of applicability.

It is suggested that, where possible, advice is provided to the user as to how best to proceed with an assessment. For instance, application of LCIA human toxicity characterisation tools for chemicals that fall outside the applicability of an applied model could be progressed by:

1. Obtaining additional relevant experimental data to be used as model input, such as intermedia partition coefficients, diffusion coefficients, etc.;
2. Identifying models applicable to the chemical under investigation and coupling outputs with LCIA input requirements;
3. Applying the 95th percentile of all available results as a default value to chemicals with missing data as incentive for getting better data; or alternatively; and
4. Omitting the chemical from the assessment, acknowledging that no information would be better than unreliable information.

However, in case a chemical is omitted from the assessment, it should be stated that the chemical could not be characterised to avoid the assumption of no-effect for such a chemical and conduct a sensitivity analysis by applying the 95th percentile across chemicals, to avoid decisions based on potentially underestimated impacts. Where deviations from standard application of LCIA tools are adopted, users should provide the appropriate documentation, enabling transparency and audibility of the overall assessment, and which would be consistent with good modelling practice (Buser et al. 2012). It is further suggested that future research prioritises developments to characterise exposure and effects associated with chemicals that fall outside the applicability domain, such as inorganic substances other than metal ions (Kirchhübel and Fantke 2019).

4.6 Characterisation factors and their uncertainty

An illustrative set of resulting human toxicity characterisation and related intermediate factors is shown in the following tables for the top 10 chemicals contributing most to the overall impact score as well as for six chemicals found in food packaging material, both related to the rice case study results presented in Section 4.7. More specifically, Table 4.4 contains human population intake fractions for chemical emissions; Table 4.5 contains product intake fractions for general population, adult, and child users for chemicals in rice

Table 4.4. Human population intake fractions for top 10 chemical substances contributing to overall impact score for the rice case study based on the data and modelling approaches proposed in the present chapter for far-field exposure.

Substance	CAS RN	Population intake fraction (iF) [kg intake/kg emitted]					
		Emission to air		Emission to freshwater		Emission to soil*	
		Inhalation	Ingestion	Inhalation	Ingestion	Inhalation	Ingestion
Parathion	56-38-2	2.0E-07	5.5E-06	5.5E-09	1.4E-04	6.2E-10	8.7E-06
Molinate	2212-67-1	5.7E-07	1.0E-05	1.7E-07	7.1E-05	5.4E-08	3.6E-05
2,3,7,8 TCDD	1746-01-6	3.9E-06	7.0E-04	4.6E-07	3.0E-03	1.2E-06**	3.2E-04**
Pendimethalin	40487-42-1	5.5E-07	3.3E-05	5.0E-08	1.6E-04	7.6E-09	1.0E-04
2,4-D	94-75-7	9.8E-07	3.3E-05	3.4E-11	1.3E-04	3.9E-11	2.3E-05
Thiobencarb	28249-77-6	5.9E-07	5.6E-05	1.5E-08	1.8E-04	3.4E-10	9.7E-07
Chloroacetic acid	79-11-8	1.3E-06	4.8E-05	2.0E-12	3.9E-05	1.5E-11	2.0E-05
Propanil	709-98-8	1.1E-06	1.3E-04	2.8E-10	1.7E-04	5.2E-12	7.4E-07
Triclopyr	55335-06-3	1.1E-06	4.2E-05	6.0E-13	1.4E-04	1.5E-12	4.8E-05
Quinclorac	84087-01-4	1.7E-06	8.1E-05	3.4E-08	1.1E-04	1.2E-07	1.1E-04

*emission to agricultural soil unless indicated otherwise; **emission to natural soil

Table 4.5. Product intake fractions for six chemical substances found in rice packaging material as defined in the rice case study (scenario US/CH) based on the data and modelling approaches proposed in the present chapter. Values in parentheses indicate lower and upper 95% confidence interval limits.

Substance	CAS RN	Product intake Fraction (PiF) [kg intake/kg in rice packaging material]					
		General population		User (adult)		User (child)	
		Inhalation	Ingestion	Inhalation or ingestion*	Dermal	Inhalation	Dermal
Diisobutyl phthalate	84-69-5	2.5E-06 (3E-07—1E-05)	9.1E-06 (1E-05—6E-06)	1.6E-03 (2E-04—7E-03)	3.1E-04 (3E-05—1E-03)	4.5E-04 (5E-05—2E-03)	4.7E-05 (5E-06—2E-04)
Dibutyl phthalate	84-74-2	2.4E-06 (3E-07—1E-05)	1.8E-05 (2E-05—2E-05)	1.6E-03 (2E-04—7E-03)	1.1E-03 (1E-04—5E-03)	4.4E-04 (4E-05—2E-03)	1.6E-04 (2E-05—7E-04)
Diisopropyl-naphthalene	38640-62-9	5.7E-06 (4E-06—1E-05)	1.6E-05 (2E-05—1E-05)	2.2E-03 (2E-04—7E-03)	9.2E-04 (8E-05—3E-03)	6.2E-04 (5E-05—2E-03)	1.4E-04 (1E-05—4E-04)
Acetyltribut-ylcitrate	77-90-7	5.3E-11 (3E-10—2E-15)	2.2E-06 (1E-05—7E-11)	8.1E-01 (6E-02—1E+00)			
Butylhy-droxytoluene	128-37-0	9.9E-10 (4E-08—3E-11)	4.2E-07 (2E-05—1E-08)	9.8E-01 (1E-01—1E+00)			
Laurolactam	947-04-6	1.8E-12 (1E-09—5E-14)	1.5E-08 (1E-05—5E-10)	1.0E+00 (2E-01—1E+00)			

*Inhalation for diisobutyl phthalate, dibutyl phthalate, and diisopropylnaphthalene, since there is no direct contact from cardboard package to food in this scenario; ingestion for tri-n-butyl acetyl citrate, 2,6-Di-tert-butyl-p-cresol, and laurolactam

packaging material; Table 4.6 contains related effects factors; and Table 4.7 finally contains characterisation factors combining (product) intake fractions and effect factors for human toxicity impacts. Product intake fractions and effect factors also include quantitative uncertainty ranges. To give insight into the particular levels of impact within each population group, product intake fractions and characterisation factors are differentiated for these groups, assuming the same linear dose-response in each group. The total impact is, in essence, the summed impact across all such population groups.

The calculation of human toxicity characterisation factors expressed in DALY/kg chemical emitted or in product (in our case in "rice packaging material") is generally based on experimental (or extrapolated) hazard data and modelled intake estimates combining fate and human exposure (Jolliet and Fantke 2015). Uncertainties in exposure estimates are mainly associated with estimates of rates of transfer among media and other environmental fate characteristics, and variability among exposed humans in the degrees and patterns of encounter with chemicals (Shin et al. 2014; Chiu et al. 2017). At a more detailed level, there is uncertainty in parameters used in estimating fate and uptake, and in the variability of exposure to people in each lumped population group, to which a single exposure level is assigned. For hazard, uncertainties arise from three main sources: uncertainty and

Table 4.6. Human cancer and non-cancer effect factors for top 10 chemical substances contributing to overall impact score and for six substances found in rice packaging material for the rice case study based on the data and modelling approaches proposed in the present chapter. Values in parentheses indicate lower and upper 95% confidence interval limits.

Substance	CAS RN	Effect factor (EF) [DALY/kg intake]	
		cancer*	non-cancer**
Parathion	56-38-2	0	96 (8—1153)
Molinate	2212-67-1		2.2 (0.2—24)
2,3,7,8 TCDD	1746-01-6	5.6E+05	3.0E+06 (3E+05—3E+07)
Pendimethalin	40487-42-1		0.03 (0.004—0.3)
2,4-D	94-75-7	0	0.07 (0.008—0.5)
Thiobencarb	28249-77-6		0.3 (0.04—2.6)
Chloroacetic acid	79-11-8	0	0.03 (0.001—0.5)
Propanil	709-98-8		0.07 (0.007—0.8)
Triclopyr	55335-06-3		0.04 (0.005—0.4)
Quinclorac	84087-01-4		0.02 (0.002—0.1)
Diisobutyl phthalate	84-69-5		0.07 (0.006—0.7)
Dibutyl phthalate	84-74-2		0.07 (0.006—0.7)
Diisopropylnaphthalene	38640-62-9		0.03 (0.003—0.2)
Acetyltributylcitrate	77-90-7		0.003 (4.2E-04—0.03)
Butylhydroxytoluene	128-37-0	3.6E-02	0.01 (0.002—0.1)
Laurolactam	947-04-6		0.03 (0.002—0.3)

*Cancer factors with "0" as value indicate that substance has been tested and shows no indication of being carcinogenic; **among the listed substances, there are none that show reproductive or developmental effects

Table 4.7. Human toxicity characterisation factors for top 10 chemical substances contributing to overall impact score and for six substances found in rice packaging material for the rice case study based on the data and modelling approaches proposed in the present chapter.

Substance	CAS RN	Human toxicity characterisation factors (CF) [DALY/kg emitted]		
		Emission to air	Emission to freshwater	Emission to soil*
Parathion	56-38-2	2.5E-03	3.2E-02	2.0E-03
Molinate	2212-67-1	1.1E-04	3.8E-04	1.9E-04
2,3,7,8 TCDD	1746-01-6	1.0E+04	2.3E+04	2.4E+03**
Pendimethalin	40487-42-1	5.3E-06	1.3E-05	8.0E-06
2,4-D	94-75-7	1.1E-05	2.0E-05	3.6E-06
Thiobencarb	28249-77-6	8.9E-05	1.5E-04	7.8E-07
Chloroacetic acid	79-11-8	6.5E-06	2.6E-06	1.3E-06
Propanil	709-98-8	4.7E-05	3.1E-05	1.3E-07
Triclopyr	55335-06-3	9.0E-06	1.5E-05	5.2E-06
Quinclorac	84087-01-4	6.6E-06	4.5E-06	4.6E-06
Substance	CAS RN	Human toxicity characterisation factors (CF) [DALY/kg in rice packaging material]		
		General population	User (adult)	User (child)
Diisobutyl phthalate	84-69-5	1.9E-06	3.1E-04	7.9E-05
Dibutyl phthalate	84-74-2	3.3E-06	4.2E-04	9.6E-05
Diisopropylnaphthalene	38640-62-9	1.4E-06	2.1E-04	5.1E-05
Acetyltributylcitrate	77-90-7	1.7E-08	6.5E-03	
Butylhydroxytoluene	128-37-0	2.8E-08	6.6E-02	
Laurolactam	947-04-6	9.6E-10	6.4E-02	

*Cancer factors with "0" as value indicate that substance has been tested and shows no indication of being carcinogenic; **among the listed substances, there are none that show reproductive or developmental effects variability in the experimental data used to derive a POD; uncertainty in the extrapolation from animal to human data; and uncertainty in the shape of the dose-response relationship (Huijbregts et al. 2005; WHO 2014; Chiu and Slob 2015). The first factor can be modelled from knowledge of the statistical distribution of the animal study databases. The animal-to-human extrapolations use default analytical models that do not include uncertainty. The dose-response modelling (proposed in the present chapter) includes uncertainty and population variability (Chiu et al. 2018). We recommend a particular choice of dose-response parameters that account for population variability and attempts to reduce uncertainty. Note that the recommended approach takes a low but not the lowest estimate of $ED10_H$, because it does not take a lower confidence bound around the lowest value derived from the experimental POD.

To the extent that calculations depend on estimates that may be uncertain, an uncertainty analysis (usually based on assessing sensitivity of calculations to alternative plausible values) is recommended (e.g., Wender et al. 2018). When the objective of analysis is the evaluation of a magnitude of potential human toxicity impact of a single activity, contributing uncertainties should be borne in mind in evaluating related human toxicity characterisation results. When, in contrast, the objective is comparison of alternative actions for their respective human toxicity impacts, many of the potential uncertainties may be calculation elements common to the compared scenarios, and they may cancel out of the comparison of final toxicity results. Further, characterisation factors can be compared to health impairments prevailing in actual populations, at best associated with chemical exposure (Landrigan et al. 2018). We presume that in many assessments, the levels of human exposure to most chemicals will be quite small compared to (potentially) a few principal chemicals and/or from other contributing factors, such as direct exposure of workers or bystanders to agricultural pesticides (Ryberg et al. 2018).

In support of comparing human toxicity characterisation results with results from other impact categories, a guiding principle is to take the best estimate and then focus on those chemicals that contribute more than, for example, one percent to the overall DALY across chemicals. In cases where substantial contributions to the overall DALY for a studied product or service is indicated, the follow-on approach is to conduct sensitivity analysis on the most influential factors for a DALY estimate, repeating the calculations with alternative values of the uncertain elements.

4.7 Rice case study application

To evaluate the presented modelling framework for characterising human exposure and toxicity effects in an LCA application context, emissions of 115 chemicals were quantified for a common rice production and processing case study that was developed as fully described in Frischknecht et al. (2016). This rice case study was originally developed to test the various updated impact categories within the Global Guidance project and is, hence, applied in the present chapter to illustrate the applicability of the discussed human exposure and toxicity

Table 4.8. Specification of rice packaging for the three rice case study scenarios. Weight fractions (wf) of chemicals in packaging material are based on Biryol et al. (2017, Table S3).

	CN	IN	US/CH
Rice packaging	1 recycled cardboard package for storing 1000 g white rice; packaging mass: 37 g; packaging area: 750 cm^2	1 low-density polyethylene (LDPE) package for storing 1000 g white rice; packaging mass: 10 g; packaging area: 670 cm^2	*Outer package:* 1 recycled cardboard package; packaging mass: 37 g; packaging area: 750 cm^2. *Inner package:* 8 low-density polyethylene (LDPE) cooking bags for storing 125 g white rice each; packaging mass: 3.5 g/bag; packaging area: 300 cm^2/bag
Storage conditions	2 months storage at 20 °C	2 months storage at 20 °C	2 months storage at 20 °C; Inner package: 20 minutes boiling at 100 °C
Packaging chemical ingredients	Diisobutyl phthalate (CAS 84-69-5), wf: 0.53%; Dibutyl phthalate (CAS 84-74-2), wf: 0.91%; Diisopropylnaphthalene (CAS 38640-62-9), wf: 0.53%	Laurolactam (CAS 947-04-6), wf: 0.53%; Acetyltributylcitrate (CAS 77-90-7), wf: 0.53%; Butylhydroxytoluene (CAS 128-37-0), wf: 0.53%	*Outer package:* chemical ingredients as in CN scenario; Inner package: chemical ingredients as in IN scenario

characterisation features, following three different scenarios. In the first scenario, rice production and processing is located in rural China and distribution and cooking in urban China (CN), in the second scenario rice production, processing, distribution, and cooking is located in rural India (IN), and in the third scenario, rice production and processing is located in rural USA and distribution and cooking in urban Switzerland (US/CH). We considered 115 chemicals that are emitted along the rice production life cycle. In order to evaluate the newly introduced product use related exposure models, the rice packaging for the three scenarios containing six additionally considered chemicals was specified as summarised in Table 4.8. More specifically, a single recycled cardboard rice package (CN), a single polyethylene rice package (IN), and multiple polyethylene rice cooking bags stored in a recycled cardboard rice package (US/CH) were used as packaging.

To compare individual chemicals across emission inventory, toxicity characterisation, and impact score levels, we have compiled ranked charts for all three aspects in Figure 4.3.

Chemical emissions per functional unit (FU, 1 kg of cooked white rice) for the 115 rice case study chemicals (cradle-to-gate) are compared with chemical emissions for the rice packaging manufacturing and disposal (Figure 4.3, left panel). Packaging related emissions indicated as '-' are typically 1 to 3 orders of magnitude smaller than the total cradle-to-gate emissions for most chemicals. Contributions of the three emission compartments (air, water, soil) are shown for the US/CH scenario. At the top of the same figure panel, mass in rice packaging material per functional unit is shown for the six chemical packaging ingredients for the US/CH scenario. Overall, emissions per FU span over 10 orders of magnitude from 0.06 µg of 4-methyl-2-pentanone emitted to freshwater in India to 1 g of propanil emitted to agricultural soil in CN and IN, with varying contributions of the different emission compartments across chemicals and scenarios. Even without combining emissions with characterisation results, it is already clear that results for human toxicity should always be shown in logarithmic scale due to the large variability across chemicals.

Human population intake fractions for chemical emissions, product intake fractions for chemical ingredients in rice packaging material, and effect factors combining human toxicity dose-response slope factors and disease severity factors (see Tables 4.4 to 4.6 for top 10 chemical substances) all contribute to the characterisation factors. Population intake fractions range from 10^{-10} µg inhaled per kg halosulfuron-methyl emitted to freshwater to 3 g ingested per kg 2,3,7,8 TCDD emitted to freshwater, spanning 16 orders of magnitude. Product intake fractions range from 0.002 µg inhaled by household members per kg laurolactam after volatilization to air during storage, to 0.99 kg ingested by adult users per kg laurolactam after migration to rice during boiling, where this chemical is used as ingredient in low-density polyethylene (LDPE) boiling rice bags. This yields a range of 12 orders of magnitude across exposure pathways and receptor populations for the same chemical. Human toxicity effect factors – derived from USEtox for cancer effects and following the approach presented in Section 4.5 for subchronic effects – span over more than 10 orders of magnitude, from 10^{-4} DALY per kg propene inhaled leading to non-cancer effects to 7 million DALY per kg 2,3,7,8 TCDD ingested leading to neurobehavioral effects. Several chemical yield 0 DALY per kg inhaled or ingested for cancer effects, meaning that these chemicals have been tested, but do not show any indication of carcinogenicity. This is in contrast to chemicals with missing data for cancer (or non-cancer) effects, which is indicated by a missing (i.e., blank) value.

(Product) intake fractions and effect factors are combined into a set of characterisation factors for human toxicity impacts across all described rice case study scenarios. Characterisation factor results for the six chemicals in rice packaging material and for the 115 chemicals emitted along the rice cradle-to-gate system are shown in Figure 4.3 (middle panel), and are aggregated into cancer and non-cancer effects and inhalation and ingestion exposure routes. For packaging ingredient chemicals, factors are expressed as DALY per kg in packaging material, and for emitted chemicals, factors are expressed as DALY/kg emitted. Significant characterisation factors are found for all six chemicals in rice packaging (ranging from 0.0003 to 0.07 DALY/kg in packaging) and for some of the 115 emitted chemicals (highest being 2,3,7,8 TCDD with 21000 DALY/kg emitted to freshwater). The characterisation factors obtained in the case study span 18 orders of magnitude and show varying contributions of effects (cancer vs. non-cancer) and exposure routes (inhalation vs. ingestion) among the selected chemicals (stacked bars in middle panel of Figure 4.3).

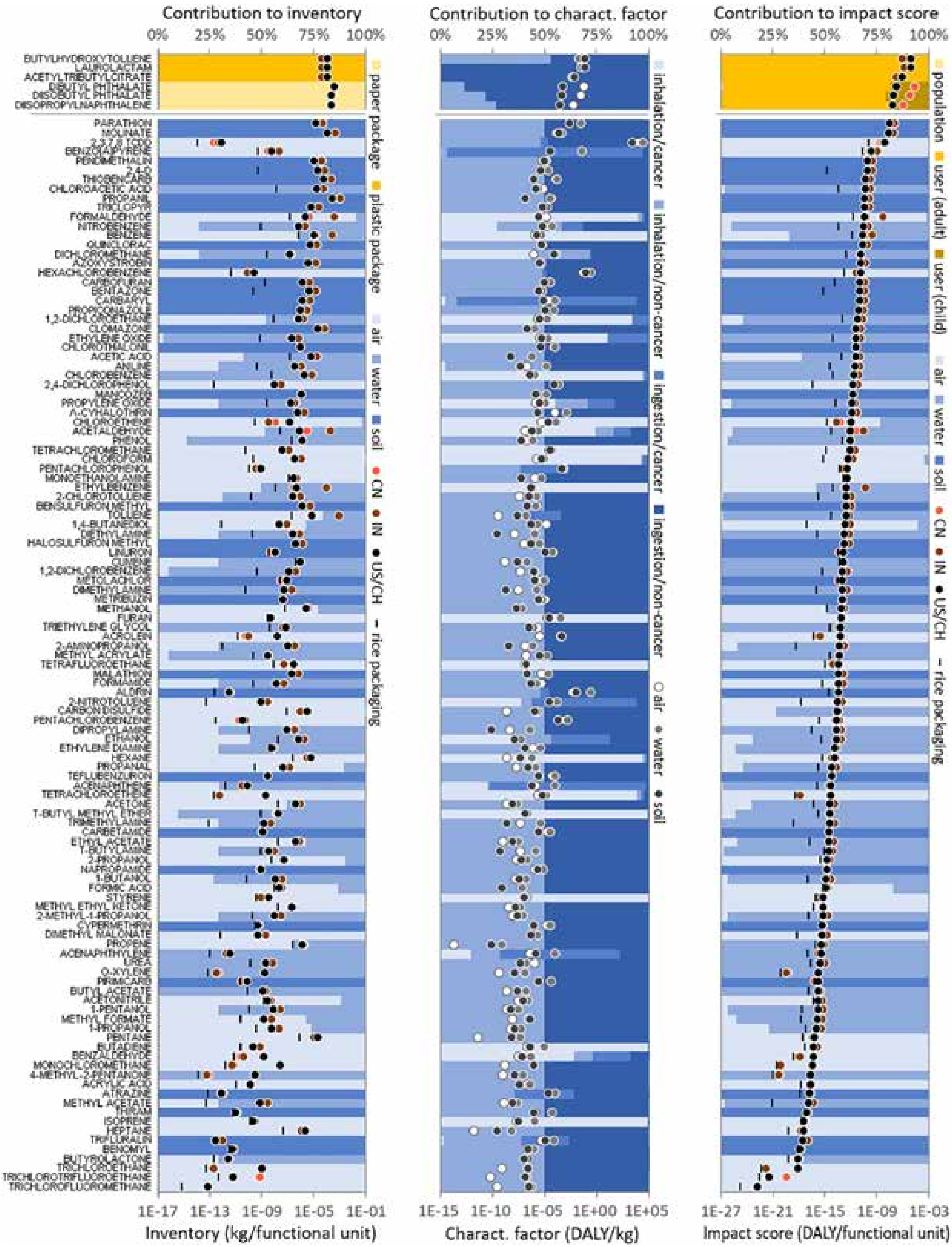

Figure 4.3. Inventory, characterisation, and impact score results for six chemicals found in rice packaging materials (top six chemicals) and chemical emitted along the cradle-to-gate of the rice case study (all other chemicals) in urban China (CN), rural India (IN), and production in United States and consumption in Switzerland (US/CH). Symbol '-' represents the level of rice packaging manufacturing and disposal emissions in relation to emissions along full cradle-to-gate for US/CH scenario. **Emission inventory in left panel:** kg in rice package/functional unit (top six chemicals) and kg emitted/functional unit (all other chemicals), contribution of packaging material (top six chemicals) and contribution of emission compartments (all other chemicals) for US/CH scenario. **Characterisation factors in middle panel:** DALY/kg in rice packaging material (top six chemicals) and DALY/kg emitted (all other chemicals) aggregated over cancer and non-cancer effects and over all exposure routes, and contribution of exposure route and effect combinations are for household population (top six chemicals) and emissions to air (all other chemicals). **Impact scores in right panel:** contribution to household population versus users (top six chemicals) and contribution of emission compartments (all other chemicals) for US/CH scenario.

Combining characterisation factors for packaging ingredients with chemical mass in packaging material as well as combining characterisation factors for chemical emissions with chemical mass emitted into air, water, and soil finally yields human toxicity impact scores that are expressed as DALY per functional unit across all considered chemicals. This means that results are directly comparable at the level of impact score between near-field chemicals in the considered product (in our case: rice packaging material) and far-field chemicals emitted along product or service life cycles. Impacts scores per chemical across the three considered scenarios are shown in Figure 4.3 (right panel), ranked according to decreasing impact scores for the US/CH scenario. Scores show that packaging ingredients are all on the upper end of human toxicity related impacts, mostly due to ingestion following contact between food packaging and food, and to a lesser extent to chemicals volatilizing from paper packages to indoor air with subsequent inhalation exposure. This highlights the importance of including direct use stage related exposure and a proper indoor environment in LCA toxicity characterisation. Impact scores range from 10^{-23} DALY for trichlorofluoromethane to 2×10^{-5} DALY for dibutyl phthalate in rice packaging material, and with that span 18 orders of magnitude.

Summing impact scores across all considered chemicals per scenario yields overall impact scores shown in Figure 4.4. Overall impact scores from cradle-to-gate range from 5×10^{-8} DALY for US/CH to 2×10^{-7} DALY for IN, dominated by emissions to soil across scenarios with various pesticides as main contributors. Rice packaging manufacturing and disposal contributes only with less than 1% to overall impact scores across scenarios, while direct use stage exposure to packaging ingredients exceeds cradle-to-gate scores by up to more than 2 orders of magnitude in the US/CH scenario, ranging from 2×10^{-6} DALY for IN to 3×10^{-5} DALY for CN. Use stage exposure is dominated by exposure of adult users via ingestion of package ingredients migrating into rice. We can finally compare our human toxicity impact scores for the rice case study with impact scores for the same case study related to fine particulate matter ($PM_{2.5}$) exposure, which were published in Fantke et al. (2016b). Overall $PM_{2.5}$ related impact scores range from 5×10^{-6} DALY for CN to 3×10^{-5} DALY for IN. With that, human toxicity impact scores driven by direct use stage exposure to packaging ingredients are in the range of impact scores for $PM_{2.5}$, further emphasizing the importance to consider near-field exposures related to the use stage in LCA. Metals and other inorganic chemicals could further contribute to human toxicity impacts, since there were not included in the present treatment of the case study, due to non-availability of updated recommended factors.

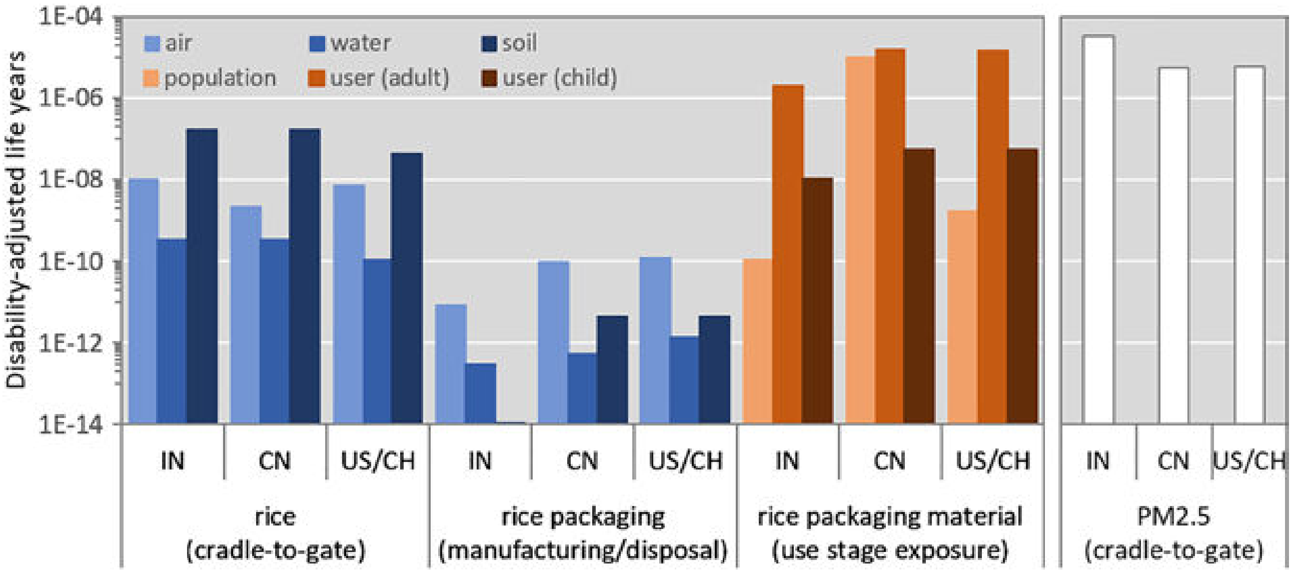

Figure 4.4. Overall impact scores (DALY) for the rice case study cradle-to-gate emissions, rice packaging manufacturing and disposal emissions, and chemical content in rice packaging material in urban China (CN), rural India (IN), and production in United States and consumption in Switzerland (US/CH). Air, water, and soil denote emission compartments and household, user (adult), and user (child) denote receptor populations for use stage related direct exposure. Right panel shows for comparison the overall impact scores from indoor and outdoor emissions of fine particulate matter ($PM_{2.5}$) and its precursors in the respective scenarios.

4.8 Recommendations and outlook

Overall, three human toxicity indicators are recommended for use in LCIA considering different severity for 'cancer', 'reproductive/developmental', and 'other non-cancer' effects. For human exposure, these indicators are recommended to build on a recently proposed matrix framework consistently coupling environmentally mediated exposures with indoor and consumer product exposures. The non-cancer indicators are recommended to build on a stochastic dose-response model proposed by the World Health Organization for a 10% population response level to derive effect factors, combined with severity factors based on the latest Global Burden of Disease statistics. To reflect on issues related to uncertainty and variability when reporting results of human toxicity impacts in LCIA, it is important to present human toxicity impact scores on a $\log_{10}$-scale, due to the substantial variability in human toxicity characterisation results across chemicals and uncertainty on characterisation factors. Moreover, we recommend to present impact scores separately for metal or metalloid compounds and organic substances, while keeping them on the same ($\log_{10}$-transformed) scale. Finally, the number of significant figures reported in characterisation results (and related impact scores) should be carefully considered and it is recommended to allow for up to two significant digits in reported impact scores (e.g., 3.4×10^{-5}) to avoid over-interpretation. Specific recommendations related to the general assessment framework, fate, exposure and dose-response modelling are detailed in the following along with suggestions for targeting future research efforts.

4.8.1 Specific recommendations for human toxicity method developers

General Recommendations:

1. Define data and model applicability domain for human exposure and toxicity characterisation and provide a flag when the applicability domain is violated.
2. Characterise uncertainty and variability, preferably quantitatively, for each calculation step of fate and exposure, toxicity effect, severity, and characterisation factors.

Fate and Exposure Assessment Recommendations:

3. Include fate and exposure processes and pathways associated with product use, extending the general framework of USEtox (Rosenbaum et al. 2008; 2011) to integrate near- and far-field exposures.
4. Use the matrix framework of direct and cumulative transfer fractions (Jolliet et al. 2015; Fantke et al. 2016a) to determine intake fractions and product intake fractions as metrics describing fate and exposure.
5. Allow flexibility for integrating models to address specific product types into the matrix framework of transfer fractions, starting with models addressing chemicals emitted indoors, or chemicals in articles or food contact materials, or on skin-surface layers or object surfaces.
6. Define default consumer product use scenarios for multiple product categories (e.g., cosmetics, building materials).
7. Distinguish the exposure of users from those of the rest of the population (including workers).
8. Add the mass of chemical in product per functional unit (derived from e.g., percent or mass fraction) to life cycle inventory (LCI) datasets.

Dose-Response Assessment Recommendations:

9. Identify a list of data sources and follow the proposed decision tree for the selection of candidate PODs for effect factor derivation.
10. Where no *in vivo* toxicity data are available, apply available QSAR models when the chemical is in the applicability domain for these models, or alternatively other new approach methods.
11. Where no *in vivo* toxicity data are available and QSAR predictions are outside their model's applicability domain, use a TTC approach, calculating the TTC-NOAEL value (TTC×100) as a screening level surrogate for the POD to avoid assigning zero toxicity to a chemical.
12. Apply state-of-science dose-response models for non-cancer effects following the WHO/IPCS approach (WHO 2014; Chiu and Slob 2015; Chiu et al. 2018). Following this approach, estimate human doses associated with a 10 percent human population response, $ED10_H$, corresponding to each POD.

13. When multiple candidate $ED10_H$ values are derived, choose the lowest as a starting point for deriving the effect factor, in line with regulatory approaches and due to lack of information regarding the most representative value for human response.
14. Extrapolate linearly from $ED10_H$ to zero to derive the effect factor.
15. For essential metals, consider only the fraction of human population that is at risk by, e.g., considering the fraction of population with biomarker level above the bioequivalent high limit corresponding to the Tolerable Upper Intake Level.
16. Refine existing non-cancer severity factor to derive two separate factors, one for reproductive or developmental health outcomes and one for all other non-cancer endpoints, and update these severity factors to reflect the most recent Global Burden of Disease incidence and DALYs (Salomon et al. 2015).

Suggestions for future consideration:

17. Apply, to the extent possible, the spatial resolution from the recommended $PM_{2.5}$ model differentiating indoor, outdoor urban, and outdoor rural settings, considering variations in exposure, toxicity, and severity.
18. Re-evaluate *in vitro* bioactivity and toxicity data for incorporation into the human effect factor derivation as mechanistic understanding and methods for use of these data are developed.
19. Re-evaluate the potential use of human epidemiological dose-response data as the science matures.
20. Extend the exposure assessment framework to also consider occupational settings and the worker population.
21. Prioritise the development of methods to characterise exposure and effects associated with inorganic substances other than metal ions.
22. Revise effect factors for cancer to harmonise with the approach used for non-cancer endpoints.

4.8.2 Specific recommendations for LCA practitioners

General Recommendations:

23. Express human toxicity related characterisation factors as DALY per unit mass emitted (for environmentally mediated exposures) or DALY per unit chemical mass in product (for consumer exposures), which can be interpreted as relative capacity to cause harm.
24. Present impact scores separately for metal or metalloid and organic substances.
25. Present total human toxicity impact scores on $\log_{10}$-scale due to the substantial variability across and uncertainty in characterisation factors.
26. Allow for up to two significant digits in reported impact scores (e.g., 3.4×10^{-5}).

4.8.3 Judgment on quality, interim versus recommended status of the factors, and recommendations

All above-listed recommendations are considered strong recommendations for current implementation, while the suggestions represent more long-term goals for improvement of human toxicity characterisation in LCIA. Factors resulting from following above-listed recommendations are considered to be of highest available quality based on state-of-the-art and robust science. However, possible differences in the recommendation status of these factors are chemical-specific and depend on the underlying uncertainty in obtaining the factors. For example, when measured toxicity data are available that were quality curated already by a regulatory authority, effect factors are "recommended." When, in contrast, effect factors were derived from TTC-NOAEL data, they have much higher uncertainty and hence are "interim recommended," i.e., still recommended for use in LCIA but associated with higher uncertainty and, hence, should be interpreted with caution when dominating overall impact scores for any given product or service system assessed. Substance results, for which data and models are outside the respective applicability domain, are likewise considered "interim recommended," i.e., recommended but to be interpreted with caution.

4.8.4 Applicability, maturity, and good practice for factors application

Applicability of all inputs and models must be considered when applying effect factors derived for human toxicity. While fate and exposure models are well developed for some types of substances, additional development to expand the chemical space may be needed for other categories, including non-metalloid inorganic substances (e.g., chlorine dioxide, sodium nitrite), per- and polyfluoroalkyl substances (PFAS), and nanomaterials. Practitioners should also consider the uncertainty and variability information available for data and models applied in the human toxicity factor derivation in their application of these factors.

4.8.5 Link to inventory databases (needs for additional inventory features, needs for additional inventory flows, classification or differentiation etc.)

To allow for calculating product intake fractions on the human exposure side, it is important and recommended that the product chemical amount (e.g., percent or mass fraction of a chemical in a specific product use) is included in life cycle inventory datasets. Otherwise, this information must be provided by the practitioner.

4.8.6 Roadmap for additional tests

While the basis for exposure factor and dose-response factor derivation is well-grounded in science and mature modelling practice for many categories of substances, case studies demonstrating the implementation of revised characterisation factors should be conducted to demonstrate the newer underlying and product type specific exposure models, as well as to examine the ability of the modelling to discriminate between different chemicals in various applications. Such efforts will inform additional evaluation and understanding of the consequences of the revisions in practice recommended in the present chapter.

4.8.7 Next foreseen steps

The next foreseen steps include going beyond the included rice case study results and calculating human exposure, effect, severity, and toxicity characterisation factors for all substances for which relevant exposure and toxicity data can be extracted from the available indicated data sources according to the recommended procedures described in this chapter. Exposure factors output will be delineated between product users and the rest of the human population. Related severity factors will be updated to reflect the most recent GBD statistics. In addition, the approaches and outcomes presented here will be published in the scientific peer-reviewed literature.

4.9 Acknowledgements

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5. Natural Resources (Mineral Resources)

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5.1 Scope

In the LCA context, natural resources include minerals and metals, air components, fossil fuels, renewable energy sources, water, land and water surface, soil, and biotic natural resources such as wild flora and fauna (Sonderegger et al. 2017). This task force had a specific focus on mineral resources excluding energy carriers (e.g., coal). In spite of numerous life cycle impact assessment methods for mineral resources, assessing the impacts of resource use continues to be a subject of debate. Even the area of protection "Natural Resources" remains controversial and it is sometimes questioned whether an impact assessment of resource use, that by definition comprises environmental and economic aspects, is within the scope of (environmental) LCA (see e.g., Drielsma et al. 2016). The lack of consensus on what actually should be protected with regard to resources in LCA (e.g., physical depletion or future extraction efforts, see e.g., EC-JRC 2010; Mancini et al. 2013; Dewulf et al. 2015), has led to the development of various impact pathways to assess the consequences of resource use. Furthermore, inadequate methods are often used, providing the "wrong" answers to the "right" questions. For example, methods assessing the long-term depletion of resources are sometimes (mis)used to assess short-term economic supply risks (Fraunhofer 2018).

To help address these challenges, the first step undertaken by this task force was to define the safeguard subject for mineral resources in the Area of Protection (AoP) "Natural Resources." The task force used an outcome of the SUPRIM project[5] (Schulze and Guinée 2018) as a starting point for the following agreed upon definition:

Within the AoP "natural resources," the safeguard subject for "mineral resources" is the potential to make use of the value that mineral resources can hold for humans in the technosphere. The damage is quantified as the reduction or loss of this potential caused by human activity. Mineral resources are chemical elements (e.g., copper), minerals (e.g., gypsum), and aggregates (e.g., sand) as embedded in a natural or anthropogenic stock.

In the following sections, the main impact mechanisms are described that are modelled by current methods to answer resource-related questions. In order to provide guidance for practitioners to select the "right" method a decision-tree has been developed (Chapter 5.4, Table 5.1). Choosing questions and the recommended impact assessment method from this decision tree will lead to greater alignment of chosen impact methods with a study's goals.

5.2 Impact mechanisms and review of approaches and indicators

Several characterisation models have been developed to connect life cycle inventory flows of mineral resources to a variety of impact indicators, which measure different aspects or impacts of natural resource use. As shown in the grey material flow layer in Figure 5.1, natural stocks of mineral resources exist within the lithosphere, with significant spatial variability in the quantity and quality of these resources. Exploration processes identify these natural resources and classify them based upon geological and economic uncertainty. Through extraction and further industrial processing these materials are transformed for use in the technosphere. They may remain within the in-use stock for a period of time before being reused, recycled, or transferred to landfills. Furthermore, materials might be dissipated at any point in the value chain (see also Section 5.7.2).

On top of the material flow layer (grey layer), an impact mechanism overview (coloured layer) has been added to show the position of reviewed characterisation models in the material flow context.

Impact mechanisms may relate the extraction of mineral resources to:

1. various indicators for the physical depletion of natural resource stocks (of different economic and geological classifications, e.g., mineral reserves, resources, or crustal content),
2. changes to resource quality and the implications of these changes, such as increasing future costs or energy demands,

5 SUPRIM (SUstainable Management of PRIMary Raw Materials through a better approach in Life Cycle Assessment) is a project by the European Institute for Innovation & Technology funded by the European Innovation Partnership on Raw Materials. The output of a SUPRIM survey was that the majority of the respondents indicated that they consider a) humans as the most relevant stakeholders valuing resources, b) the technosphere as the system of concern (although some minerals in the ecosphere also provide an value for humans, e.g., sand filtering groundwater), and c) both primary and secondary supply chains as relevant production systems (see Berger et al. 2019).

3. economic externalities (based on mineral resource economics and not on resource quality changes), or
4. the extraction of the exergy content of mineral resources.

Within the technosphere, the provision of raw materials may be associated with potential supply risks, represented by potential supply disruptions arising from geopolitical and market factors (e.g., political stability of mining countries or company concentration), as well as the vulnerability of material users to these disruptions. Additional aspects of the material stocks and flows could be of high interest to quantify, but they are currently hardly accounted for within LCI and LCIA, such as dissipative losses of materials and the resulting "dilution of total stocks."

A literature review identified 27 impact assessment methods of resource use in Life Cycle (Sustainability) Assessment (LC[S]A). These existing approaches are classified into four method categories based on the main impact mechanisms illustrated in Figure 1 (see also Figure 2): depletion, future efforts, thermodynamic accounting, and supply risk methods. The methods include both midpoint and endpoint approaches, which model impacts at the middle or at the end of the cause-effect-chain, respectively.

5.2.1 Depletion methods

The depletion concept concerns the reduction of a resource stock (or a set of stocks). This concept is often used as a proxy for the accessibility of resources.

The Abiotic Depletion Potential (ADP) model (Guinée and Heijungs 1995; van Oers et al. 2002) is based on this concept and expresses the accessibility of resources with the ratio of the current extraction rate to (the square of) the size of the natural stock (i.e., economic reserves, reserve base, or ultimate reserves). The Swiss Ecological Scarcity Method (Frischknecht and Büsser Knöpfel 2013) uses the ADP model. The Anthropogenic stock extended Abiotic Depletion Potential (AADP) model (Schneider et al. 2011, 2015) considers anthropogenic stocks within the technosphere in addition to natural stocks. Environmental Development of Industrial Products (EDIP) 1997 (Wenzel, Hauschild, and Alting 1997) and 2003 (Hauschild and Potting 2005) and Life-cycle Impact assessment Method based on Endpoint

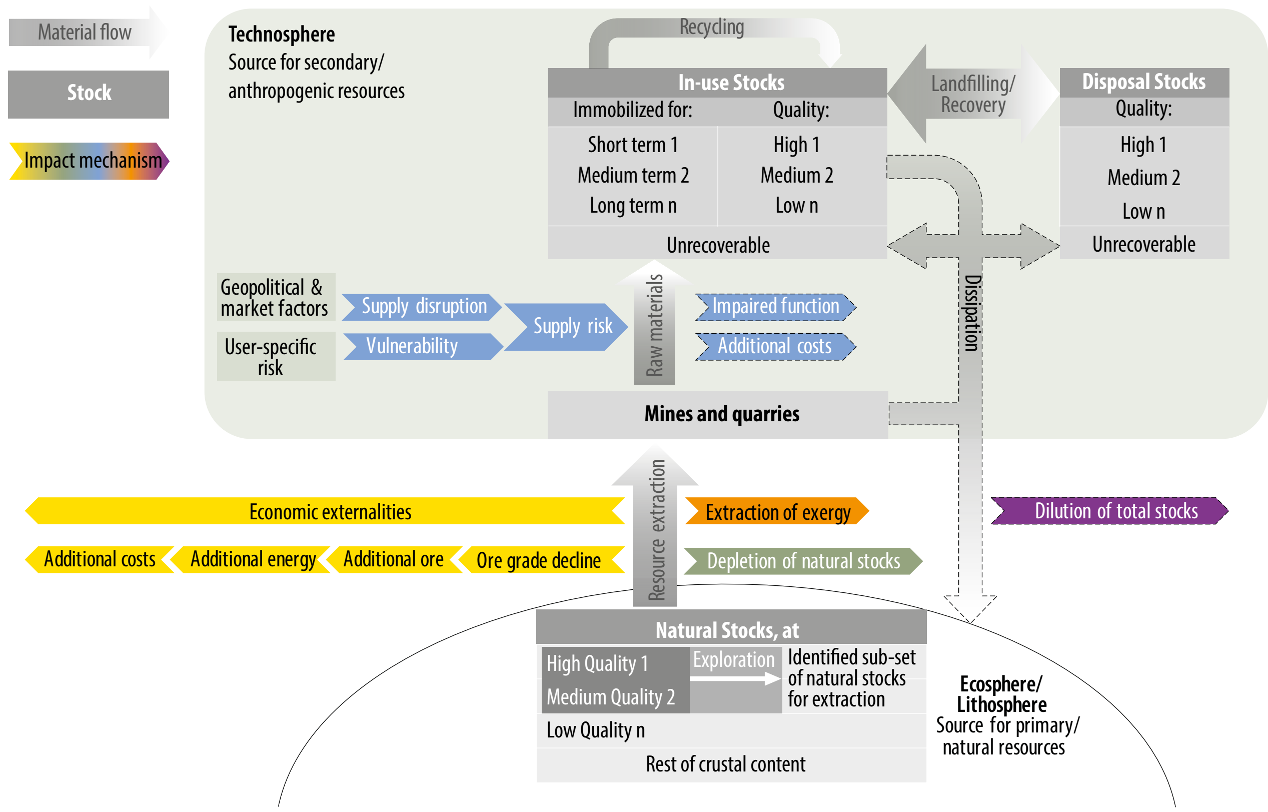

Figure 5.1. Material flow (grey layer) and impact mechanisms overview, presented in colour for depletion methods (green), future effort methods (yellow), thermodynamic accounting methods (orange), supply risk methods (blue), and the "dilution of total stocks" approach (purple). Dashed material flows and impact mechanisms are proposed or discussed but not agreed, operational, or published yet (Figure from Sonderegger et al. 2019).

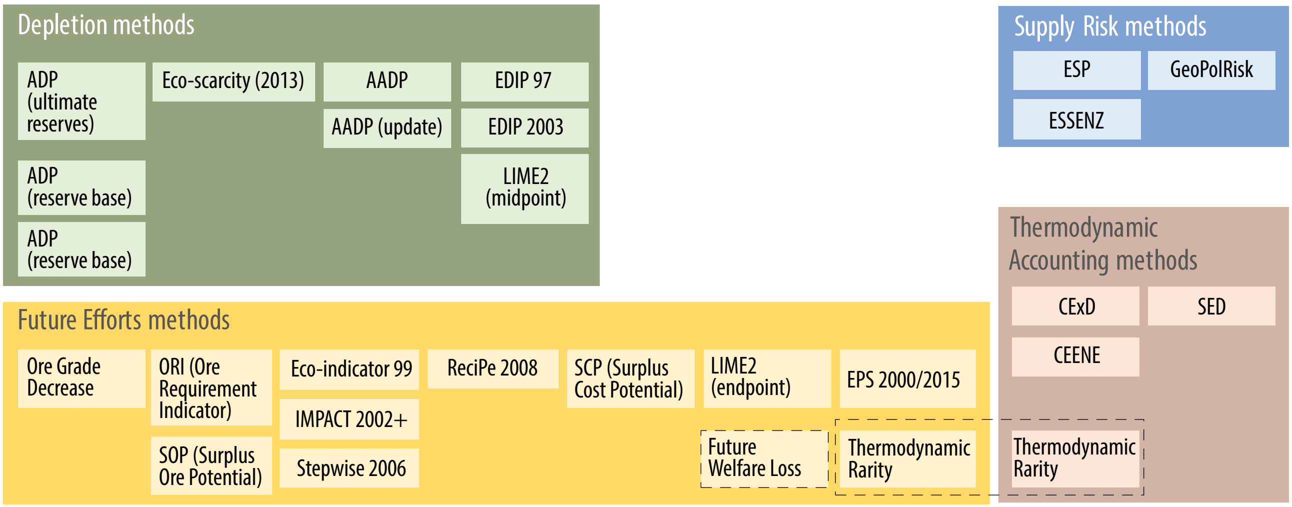

Figure 5.2. Overview of methods categorisation according to underlying impact mechanisms; the Future Welfare Loss approach is shown in a dashed box since it has not been published at the time of the Pellston Workshop; the thermodynamic rarity approach has elements of two categories (Figure from Sonderegger et al. 2019).

modelling (LIME2) (midpoint) (Itsubo and Inaba 2012) are conceptually different from ADP-based methods, i.e., they only consider the inverse of the size of the natural stock and not the ratio of the extraction rate to the stock.

5.2.2 Future efforts methods

Future efforts methods may be generalised as seeking to assess the consequences of current resource use on future societal efforts. These may include increased efforts to extract a unit of mineral resource in the future or increased economic externalities, which can be driven by the change of resource quality. Only one method, the Ore Grade Decrease method (Vieira et al. 2012), provides characterisation factors (CFs) that directly quantify the decrease of ore grade due to resource extraction. Several closely related methods focus on the consequence of quality change by means of:

1. surplus extraction requirement of ore (Ore Requirement Indicator [Swart and Dewulf 2013], Surplus Ore Potential [Vieira et al. 2016a], as used in ReCiPe2016 [midpoint] [Vieira et al. 2016b], and LC-Impact [Vieira and Huijbregts 2016]);
2. surplus energy (Eco-indicator 99 [Goedkoop and Spriensma 2001], as used in Impact 2002+ [Jolliet et al. 2003] and Stepwise [Weidema et al. 2008; Weidema 2009]); and
3. surplus cost (ReCiPe 2008; Surplus Cost Potential [Vieira, Ponsioen et al. 2016]; ReCiPe 2016 [endpoint] [Vieira et al. 2016b]).

EPS 2000/2015 (Steen 1999, 2016) and Thermodynamic Rarity (Valero and Valero 2015) assess average cost and exergy, respectively, for mining elements from an assumed average crustal concentration, which can be interpreted as a far-future state. They do not consider the change of resource quality. Apart from these methods, the Future Welfare Loss method[6] and LIME2 method (Itsubo and Inaba 2012, 2014) assess the externality of resource use especially for future generations.

5.2.3 Thermodynamic accounting methods

Thermodynamic accounting methods quantify the cumulative exergy (or energy) use in a product system. In this group, we included the following methods: cumulative exergy extraction from the natural environment (CEENE) (Dewulf et al. 2007; Alvarenga et al. 2013; Taelman et al. 2014); the cumulative exergy demand (CExD) (Bösch et al. 2007; Hischier et al. 2009); thermodynamic rarity (TR) (Valero and Valero 2015); and solar energy demand (SED) (Rugani et al. 2011). For metals and minerals, exergy methods account for a) the difference between the exergy of these resources as found in nature and as found in a defined reference state (CEENE and CExD) or b) the exergy

6 The Future Welfare Loss method suggested by De Caeval et al. (2012) was discussed extensively in this task force prior to the Pellston Workshop but the method has only been published after the workshop in Huppertz et al. (2019). The approach assesses the future loss in welfare assessed directly in monetary terms as the difference between the social and private value of the extracted resource, calculated as the net present value with the social and private discount rates, respectively.

replacement cost[7] (TR); while the SED accounts for the solar energy required for the formation of natural stocks of mineral resources.

5.2.4 Supply risk methods

Outside the LCA community, several methods have been developed to assess the "criticality" of raw materials (see e.g., Erdmann and Graedel 2011; Achzet and Helbig 2013), which consider e.g., socio-economic and/or environmental aspects in addition to geologic accessibility constraints. The concept of criticality (called supply risk in this report) typically includes considerations of supply disruptions of raw materials and the vulnerability of a user to such disruptions (compare Figure 5.1).

To operationalise the consideration of supply risks in LCA, three methods have been developed: the geopolitical supply risk (GeoPolRisk) method (Gemechu et al. 2015; Helbig et al. 2016; Cimprich et al. 2017); the economic scarcity potential (ESP) method (Schneider et al. 2014), and the integrated method to assess resource efficiency (ESSENZ) (Bach et al. 2016), which is effectively an extension and update of the ESP method.

It should be noted, that these supply risk methods have a different perspective than "traditional" LCIA methods: they do not assess impacts of a product system on the environment (inside-out perspective). Instead, they assess supply constraints resulting from the global production system on the product system under study (outside-in perspective).

5.3 Process and criteria applied and process to select the indicator(s)

The 27 impact assessment methods were assessed based on 47 criteria (e.g., about underlying concepts, scientific robustness, or transparency), developed in an earlier phase of the Life Cycle Initiative consensus finding process (see the Supplementary Material from Sonderegger et al. 2019). Additionally, the methods were implemented in an electric vehicle LCA case study, in which it was possible to identify different results across the different methods, highlighting the consequences of various methodological choices (including different approaches or different sources of data to feed CF). Furthermore, the 27 methods were compared with the safeguard subject. The key findings and initial recommendations of this task force were presented in a white paper.

At the Pellston Workshop, the participants (six active and two passive task force members) established a list of key questions an LC(S)A practitioner would be interested in, when assessing impacts on resource use. The methods were then assigned to questions and assessed by their capability to answer them, based on (a) the modelling approach, (b) the underlying data used, (c) the coverage of characterization factors (CFs), and (d) the degree to which existing methods are compatible with this definition of the safeguard subject. The most appropriate method(s) for the specific questions were then recommended. Non-operational LCIA methods were not considered. The limitations of the chosen or recommended methods were debated to support the decision to indicate the level of recommendation (e.g., interim recommendation). Improvements to these methods were also proposed.

Moreover, to support the user of the LCIA method(s), the task force highlighted which questions are more related to environmental LCA and which ones are more related to other sustainability issues in a life cycle perspective.

5.4 Description of indicator(s) selected

As mentioned in Section 5.1, different stakeholders might have different questions with regard to the assessment of resource use in LCA. As shown in table 5.1, these questions either address the impacts of a product system's resource use on the opportunities of future generations to use resources (inside-out) or resource availability for a product system (outside-in). We recommend using the inside-out related questions within environmental LCA and the outside-in related questions within broader life cycle-based approaches,

7 The exergy replacement cost is defined as the exergy that would be needed to extract a mineral from Thanatia (a theoretical state of the earth crust in which all mineral resources are completely dispersed) (Valero and Valero 2015) to the conditions of concentration and composition found in the mine, using prevailing technology.

such as LC(S)A[8]. These two basic questions can be divided into sub-questions and answered by different LCIA methods as shown below.

We could not reach consensus on which of the inside-out related questions are more relevant to LCA. We suggest that the LCA practitioner considers the goal

Table 5.1. Questions related to the impacts of mineral resource use and matching recommended methods including the level of recommendation. Colours of the questions indicate the link of the question to the four method categories defined in Figure 5.2: green – depletion methods, yellow – future efforts methods, orange – thermodynamic accounting methods, blue – supply risk methods.

How can I quantify the relative…

...changing opportunities of future generations to use mineral resources due to a current mineral resource use? (inside-out)					….potential mineral resource availability issues for a product system? (outside-in)	
...contribution of a product system to the depletion of mineral resources?	...contribution of a product system to changing mineral resource quality?	...consequences of the contribution of a product system to changing mineral resource quality?	...(economic) externalities of mineral resource use?	…impacts of mineral resource use based on thermo-dynamics?	...potential availability issues for a product system related to mid-term physico-economic scarcity of mineral resources?	...potential accessibility issues for a product system related to short-term geopolitcal and socio-economic aspects?
$ADP_{ultimate\ reserves}$	Ore Grade Decrease	SOP	LIME2 (endpoint)	CEENE	$ADP_{economic\ reserves}$	ESSENZ
$ADP_{reserve\ base}$		ORI	Future Welfare Loss*	CExD	$ADP_{reserve\ base}$	GeoPolRisk
$ADP_{economic\ reserves}$		Eco-Indicator 99		TR	Eco-sWcarcity	ESP
Eco-scarcity		Impact 2002+		SED	AADP	
AADP		Stepwise 2006			AADP (update)	
AADP (update)		ReCiPe 2008			EDIP 97	
EDIP 97		SCP			EDIP 2003	
EDIP 2003		EPS			$LIME2_{midpoint}$	
$LIME2_{midpoint}$		TR-ERC				**Interim recommended**
Recommended		**Interim recommended**	**Interim recommended**	**Interim recommended**	**Suggested**	**Suggested**

Abreveations: ADP: Abiotic Depletion Potential, AADP: Anthropogenic stock extended Abiotic Depletion Potential, ORI: Ore Requirement Indicator, SOP: Surplus Ore Potential, SCP: Surplus Cost Potential, TR: Thermodynamic Rarity, TR-ERC: Thermodynamic Rarity - Exergy Replacement Cost, CExD: Cumulative Exergy Demand, CEENE: Cumulative Exergy Extraction from the Natural Environment, SED: Solar Energy Demand, ESP: Economic Scarcity Potential, ESSENZ: Integrated Method to Assess Resource Efficiency, GeoPolRisk: Geopolitical Supply Risk

* The Future Welfare Loss method was not published at the time of the Pellston Workshop and, thus, could not be recommended. However, it models a relevant complementary impact pathway to the one described by LIME2 (endpoint) and this was discussed in detail prior to the workshop within the task force.

Table 5.2. Scopes of recommended indicators

	$ADP_{ultimate\ reserves}$	SOP_{URR}	$LIME2_{endpoint}$	CEENE	$ADP_{economic\ reserves}$	ESSENZ	GeoPolRisk
Geographical resolution/ perspective	Global	Global	Global	Global	Global	Global	Country
Timeframe of impacts	More than decades to hundreds of years	More than decades to hundreds of years	More than decades to hundreds of years	Current change	A few decades	Current accessibility	Current accessibility
Users affected	Future users	Current users	Future users	Current users	Next few generations	Current users	Current users
Number of CF for mineral resources (metals & metalloids / non-metal elements / minerals & aggregates)	49 (44/5/0)	75 (45/4/26)	19 (19/0/0)	65 (23/2/40)	42 (39/3/0)	49 (41/4/4)	32 (21/4/7)
Number of CF for energy carriers / other resources (water, land use, biotic resources, inter-mediates, etc.)	4/0	0/0	4/0	4/12	4/0	4/7	1/13

8 Minority statement about classification of questions: One participant did not agree with the classification of questions. The participant expressed that outside-in related questions are still within the scope of environmental LCA. However, this depends on the definition of "the environment." Human health is generally included in the traditional LCA, therefore human life and well-being can be a part of the environment. A product system provides a value for supporting human well-being.

and the scope of the LCA study in order to determine the relevance of the question to the assessment. Similarly, we could not reach consensus on which of the outside-in related questions is most relevant to broader life cycle-based approaches. Thus, the level of recommendation denotes how well the recommended method can answer the respective question and should not be interpreted as an absolute judgement.

In order to analyse the various impacts of resource use on different aspects of the safeguard subject, a broad set of the recommended LCIA methods can be applied. If the practitioner simply selects the method with the highest recommendation level ($ADP_{\text{ultimate reserves}}$), he or she should be aware that the result is the answer to a specific question (see table 5.1).

Table 5.2 provides more information about the geographic resolution, the timeframe of impacts, and the affected users as represented by the recommended methods.

Question: How can I quantify the relative contribution of a product system to the depletion of resources?

Recommended method: $ADP_{\textbf{ultimate reserves}}$ (CML 2016)[9]

Level of recommendation: Recommended

Generally, the ADP model relates annual extraction rates to a stock estimate. Depletion is assessed as extraction rate (E) divided by stock estimate (R) and this ratio is multiplied by 1/R to account for differences in stock size as shown in Equation 1 (see Guinée and Heijungs [1995] for a detailed discussion of modelling choices). Furthermore, the ADP is defined relative to the reference substance antimony[10]. Equation 1 shows the calculation of the ADP (which is at the same time the CF) for a resource *i* relative to the reference substance antimony (*ref*). For $ADP_{\text{ultimate reserves}}$ the stock estimate *R* is the ultimate reserve (crustal content).

$$ADP_i = CF_i = \frac{E_i/R_i}{E_{ref}/R_{ref}} * \frac{1/R_i}{1/R_{ref}} = \frac{E_i/R_i^2}{E_{ref}/R_{ref}^2} \qquad (1)$$

According to Guinée and Heijungs (1995), the ultimately extractable reserve is the only relevant stock estimate with regard to depletion of natural stocks. However, it will never be known because it depends on future technological developments. Therefore, a proxy is needed and ultimate resources (crustal content) is considered to be a better proxy than fluctuating stock estimates such as resources or economic reserves as defined by the U.S. Geological Survey (USGS), which provide more of a mid-term perspective (a few decades). Alternatively, a simpler model without extraction rates such as used in EDIP or LIME2 (midpoint) could be used. However, these methods do not provide CFs using crustal content but economic reserves (although they could be easily calculated). While we recommend using $ADP_{\text{ultimate reserves}}$ as the baseline method, we also suggest, following the method developers van Oers et al. (2002), to use other depletion methods for sensitivity analysis.

With regard to depletion of natural stocks, the model is valid. However, the need to use a proxy for the ultimately extractable resource is a limitation. With regard to depletion of total (natural and anthropogenic) stocks, further limitations should be acknowledged. Firstly, by considering extraction rates, the method is not able to distinguish the part of the resource that is occupied by use but might be re-used in the future, and the part that economically and/or technically cannot be recovered, i.e., that is dissipatively lost (the issue of dissipation is further discussed in Section 5.7.2). Second, by considering the crustal content as a resource stock, anthropogenic stocks are not explicitly taken into account. However, it can be argued that the anthropogenic stocks are implicitly included (there is no deduction of already extracted resources from ultimate reserves) although they are not explicitly quantified. Therefore, as long as the concept of dissipation is not implemented, the $ADP_{\text{ultimate reserves}}$ method might be interpreted as the best available proxy for depletion of the total resource stock and therefore is a recommended method[11].

Question: How can I quantify the relative contribution of a product system to changing resource quality?

Recommended method: None

This question refers to modelling approaches that would evaluate a change in a resource quality without considering any consequences of it. Only

9 An update of the recommended ADP method is under review but not yet available at the time this report is finalised.

10 The choice of the reference substance was arbitrary (see Guinee et al. 1995)

11 Minority statement about level of recommendation: Two participants did not agree with the level of recommendation of ADP ultimate reserve. Since the method focuses on the extraction and stocks of natural resource only and neglects anthropogenic stocks and dissipation rates, they felt the level should rather be "interim recommended" until these deficiencies are addressed.

one matching method was identified, i.e., ore grade decline (Vieira et al. 2012), which is operational only for copper and therefore is not recommended. Moreover, methods answering the follow-up question, "How can I quantify the consequences of the contribution of a product system to changing resource quality?" can be interpreted as proxy for the question discussed here, depending on modelling choices. For instance, ORI and SOP quantify the amount of surplus ore required to mine the same amount of metal, i.e., the consequence of a quality change.

Question: How can I quantify the relative consequences of the contribution of a product system to changing resource quality?

Recommended method: SOP_{URR} (Ultimate Recoverable Resource) (Vieira 2018)

Level of recommendation: Interim recommended

The surplus ore potential (SOP) (Vieira et al. 2016a) measures the average additional ore required to produce the resource in the future, based upon resource grade-tonnage distributions and the assumption that higher grade ores are preferentially extracted.

A log-logistic relationship between ore grades and cumulative extraction is developed for each resource 'x' based upon fitting regression factors (α_x and β_x) to the observed (A_x; kg_x) grade-tonnage distribution of deposits. Prior to this procedure, an economic allocation of ore tonnage is performed to account for potential co-production. An average characterisation factor is developed by integrating along the product of resource extraction (RE_x) and the inverse of the grade log-logistic relationship (OM_x; the amount of ore mined per amount of resource x) from cumulative

$$SOP_x = \frac{\int_{CRE_{x,total}}^{MRE_x} OM_x(RE_x)\, dRE_x}{R_x},$$

where

$$OM_x = \frac{1}{G_x} = \frac{1}{exp(\alpha_x)\left(\frac{A_{x,sample}\text{-}CRE_{x,sample}}{CRE_{x,sample}}\right)^{\beta_x}} \qquad (2)$$

resource extraction (CRE_x) to the maximum resource extraction (MREx) then dividing by total remaining extraction (R_x). Therefore, the CF representing the average surplus ore potential of each resource (SOP_x; kg_{ore} per kg_x) can be expressed as:

As the total remaining extraction is unknown, this is approximated as being equivalent to demonstrated economic reserves and ultimate recoverable resource (URR, approximated as 0.01% of the resource within 3 km) to provide two sets of characterisation factors ($SOP_{reserves}$ and SOP_{URR}). Vieira (2018) extended a set of CFs for 18 resources based on the approach described above (Vieira et al. 2016a) to 75 resources through the extrapolation of SOP values based upon a correlation between SOP and resource prices.

Other methods were not recommended for the following reasons: ReCiPe2016 endpoint is based on 'surplus cost potential' (SCP) and uses a mid-to-endpoint conversion factor based on copper, which may not be applicable to all resources. The original SCP method (Vieira, Ponsioen et al. 2016) and the ore requirement indicator (ORI) method were also not selected as they are based upon regression data that was determined using mined ore tonnage and mining cost data over a period characterised by very high growth in mineral demand and mineral price increases that significantly distorted short-term mineral markets. ReCiPe2008 is based on data for existing mines only and includes no data for undeveloped mineral deposits known to be available. Eco-Indicator 99, Impact2002+, Stepwise2006, EPS 2000/2015, and thermodynamic rarity methods do not fully address the question as the resource quality change associated with extraction is not modelled and we therefore do not recommend them.

A key limitation of the SOP_{URR} is that it is assuming mining from highest to lowest grade and not explicitly accounting for competing factors such as technology and economic considerations (Sonderegger et al. 2019). This, as well as the extrapolation of observed grade-tonnage data, is an assumption for the long-run future and therefore impossible to prove or falsify. Therefore, the SOP_{URR} method as implemented Vieira (2018) is given a recommendation level of 'interim recommended.'

Question: How can I quantify the relative (economic) externalities of resource use?

Recommended method: LIME2 (endpoint)

Level of recommendation: Interim recommended

The LIME2 method (endpoint) is based on El Serafy's user cost (El Serafy 1989). The user cost assesses the share of the economic value of extracted resources that need to be reinvested to maintain the benefit given from the extraction of resources (Itsubo and

Inaba 2014). The indicator of LIME2 (endpoint) expresses this user cost as the economic externality of resource use in the unit of monetary value and is calculated as follows:

$$\text{CF LIME2 method (Endpoint)} = R\{1/(1+i)N\}/P \qquad (3)$$

where **R** is annual profit of the target element; i is the interest rate; **N** is ratio of reserve to production (years to depletion); **P** is current annual production amount of the target element.

The LIME2 method was recommended since it incorporates uncertainty data and was the only peer-reviewed method available in this category at the time of the Pellston Workshop. A few months later, the future welfare loss method was published (Huppertz et al. 2019), which describes a relevant complementary impact pathway to the one modelled in LIME2. While LIME2 tries to assess the excessive benefit obtained by current users, which should be reduced to share the values with future users, the future welfare loss method aims at assessing the lost value of resources resulting from an underestimation of the current market price, which does not fully consider a resources future value.

However, the main limitations of the LIME method are the arbitrariness of selecting an interest rate, relevance of assessing economic aspect in environmental LCA, and applicability of the El Serafy's method to a specific mineral. From this point of view, the method recommendation level is "interim recommended."

LIME method has three versions (LIME/LIME2/LIME3). LIME2 (interim recommended for this question) is the updated version of LIME with the inclusion of uncertainty analysis. LIME3, which was not published at the time of the Pellston Workshop, is an extended version with country-specific CFs for all targeted minerals, while LIME and LIME2 provide generic CFs without consideration of differences in production and reserve in a country.

Question: How can I quantify the mineral resource use based on thermodynamics?

Recommended method: CEENE

Level of recommendation: Interim recommended

The exergy of a resource is the maximum amount of useful work that can be obtained from it when it is brought to equilibrium with the environment (reference state). As resources (in minerals) differ from the reference state with respect to their chemical composition and their concentration, in principle they can produce work. Although most metal and mineral resources are not extracted from nature with the aim to directly produce work, they still contain exergy. For example, the copper in a copper deposit is much more concentrated and occurs in another chemical form (e.g., $CuFeS_2$) than copper dissolved in seawater (the reference state for copper). This distinction with respect to commonness makes a resource to be valuable in exergy terms.

The cumulative exergy extraction from the natural environment (CEENE) method (Dewulf et al. 2007; Alvarenga et al. 2013; Taelman et al. 2014) aggregates the exergy embedded in extracted resources (e.g., copper), measured as the exergy difference between a resource as found in nature and the defined reference state in the natural environment. Using the definition of Szargut et al. (1988) the reference state is represented by a reference compound that is considered to be the most probable product of the interaction of the element with other common compounds in the natural environment and that typically shows high chemical stability (e.g., SiO2 for Si) (De Meester et al. 2006). For metals, CEENE calculates the exergy value of the mineral species (e.g., CuFeS2) containing the target metal, making it independent of the ore grade.

The Pellston Workshop participants recommend the CEENE method over other thermodynamic accounting methods because it was originally operationalised to LCA by proposing a more accurate exergy accounting method than the one used in the cumulative exergy demand (CExD) method. For instance, in CExD the exergy values of metals are calculated from the whole metal ore that enters the technosphere, whereas CEENE only regards the metal-containing minerals of the ore (with the argument that the tailings from the beneficiation are often not chemically altered when deposited). While thermodynamic rarity (TR) offers an alternative reference state (Thanatia) and as opposed to the other approaches considers ore grade in the evaluation of resources, it is not mature enough when compared to Szargut et al.'s (1988) approach (used in CEENE).

Another method with a thermodynamics-based approach is the solar energy demand (SED), which is based on the emergy approach (with a few differences in the calculation approach) (Rugani et al. 2011). It considers the equivalent solar energy that nature requires to provide a resource, which includes more energy than can be used out of this resource. Therefore, the method is less relevant than CEENE with regard to the safeguard subject of mineral resources. As the focus of this work is on mineral resources and the overall concern is "changing opportunities of future generations," the recommendation level was "interim recommended." The rationale is that, even though CEENE allows quantifying the value of a resource in exergy terms, the approach, as currently applied to metals and minerals does not fully reflect why society values metals, as it leaves aside non-thermodynamic aspects.

Question: How can I quantify potential resource availability issues for a product system related to physico-economic resource scarcity?

Recommended method: $ADP_{economic\ reserves}$

Level of recommendation: Suggested

The model for calculation of $ADP_{economic\ reserves}$ is the same as in equation (1) but with the economic reserves as the stock estimate *R*. The (economic) reserves are the part of known resources that is judged to be economically extractable at a given point in time. The extraction-to-stock ratio used in the model can be interpreted as a scarcity measure and accordingly the CFs of $ADP_{economic\ reserves}$ as a measure of the pressure on the availability of primary mineral resources.

The extraction rates are considered to be important in this mid-term perspective (a few decades), which is why a model excluding extraction rates – as used in EDIP and LIME2 (midpoint) – is not recommended here.

The exclusion of anthropogenic stocks in models addressing the abovementioned question is considered to be a major limitation because they can strongly influence the "resource availability for a product system" (Schneider et al. 2011). Opposite to $ADP_{ultimate\ reserves}$ – anthropogenic stocks are not implicitly included in the natural stock estimate used in $ADP_{economic\ reserves}$. Existing attempts to include anthropogenic stocks in the characterisation models (AADP [Schneider et al. 2015]) face the challenge of not considering how much of this stock would become available within the time horizon implied by the CFs.

Furthermore, the use of the economic reserves estimate is problematic because it has actually grown in absolute numbers in the past and the extraction-to-economic-reserve-ratios have been more or less stable, so no increasing scarcity could be observed. Furthermore, the economic reserve estimates are highly uncertain for by-products. Finally, the method has not been developed to explicitly answer an outside-in question, which is why the results need be interpreted carefully. For these reasons, the recommendation level for $ADP_{economic\ reserves}$ is "suggested."

Question: How can I quantify potential resource accessibility issues for a product system related to short-term geopolitical and socio-economic aspects?

Recommended methods: ESSENZ and GeoPolRisk

Levels of recommendation: Interim recommended and suggested, respectively

Table 5.3. Excerpt of CFs for the selected methods for six mineral elementary flows

	$ADP_{ultimate\ reserves}$	SOP_{URR}	$LIME\ 2_{endpoint}$	CEENE	$ADP_{economic\ reserves}$	ESSENZ	GeoPolRisk (EU-28)
Mineral Resource	kg Sb-eq/kg	kgOre/kg	Yen/kg	MJexergy/kg	kg Sb-eq/kg	1/kg	-
Cobalt	1.6E-05	9.6E+01	#N/A	1.2E+00	4.9E-02	1.4E+11	#N/A
Copper	1.4E-03	1.5E+01	1.0E+02	1.6E+01	3.9E-03	4.6E+07	9.3E-02
Gold	5.2E+01	5.5E+04	6.7E+05	7.8E-02	4.0E+01	1.9E+12	5.1E-02
Iron	5.2E-08	9.1E-01	1.5E-01	3.6E-01	3.6E-06	2.0E+06	6.8E-04
Lithium	1.1E-05	7.1E+01	#N/A	#N/A	4.4E-02	1.0E+11	#N/A
Magnesium	2.0E-09	1.2E+01	#N/A	#N/A	#N/A	3.8E+08	4.7E-01
Nickel	6.5E-05	4.2E+01	3.6E+02	2.5E+01	1.7E-02	3.2E+09	4.6E-02
Silver	1.2E+00	2.2E+03	1.4E+04	3.3E+00	8.2E+00	2.5E+11	3.8E-02
Tantalum	4.1E-05	7.7E+02	#N/A	2.6E-01	2.3E+01	1.5E+13	#N/A
Tellurium	4.1E+01	2.7E+02	#N/A	#N/A	1.1E+01	4.7E+13	#N/A
Gravel	#N/A	#N/A	#N/A	9.0E-02	#N/A	2.1E+07	#N/A
Metamorphous rock, graphite containing	#N/A	#N/A	#N/A	3.4E+01	#N/A	#N/A	#N/A

The ESSENZ method (Bach et al. 2016), which enhanced the preceding ESP method (Schneider et al. 2014), provides CFs for 49 metals and four energy carriers quantifying 11 geopolitical and socio-economic accessibility constraints (country concentration of reserves and mine production, price variation, co-production, political stability, demand growth, feasibility of exploration projects, company concentration, primary material use, mining capacity, trade barriers). Indicators for these categories are determined and divided by a target threshold above which accessibility constraints are assumed to occur. Subsequently, this distance-to-target (DtT) value is normalised by the global production of the respective resource to consider that the accessibility constraints described above can be more severe for resources produced in relatively low amounts. Finally, the normalised DtT factors are scaled (to a range between 0 and 1.73×10^{13} in each category) to balance the influence of the LCI and the CFs on the LCIA result.

The GeoPolRisk method (32 CFs) weighs the political stability of upstream raw material producing countries by their import shares to downstream product manufacturing countries. It incorporates the country concentration of reserves as a mediating factor in supply disruption probability arising from political instability of trade partner countries. The logic is that highly concentrated production of raw materials limits the ability of importing countries to restructure trade flows in the event of a disturbance (such as political unrest) that may lead to supply disruption. Domestic production is assumed to be "risk-free" from a geopolitical perspective. Further, a "product-level importance" factor that effectively cancels out the magnitude of inventory flows is considered and "substitutability" of inventory flows as a risk mitigation factor, using semi-quantitative indicator values incorporated in the method.

Comparing the two approaches, ESSENZ considers more potential geopolitical and socio-economic constraints and provides more CFs. In contrast, GeoPolRisk allows for considering the specific import structure of a particular country.

Considering the individual strengths of the two approaches, the ESSENZ method is interim recommended to assess the supply risk of multinational companies having locations all over the world. The GeoPolRisk method is suggested to assess country-specific supply risks arising from political instability of trade partners from which resources are imported.

Both recommended methods rely on the key assumption that supply risk is a function of supply disruption probability and vulnerability. They share the limitation of focusing on the supply risk of primary resources only, and either do not consider the country-specific import situation (ESSENZ) or are limited concerning the accessibility constraints considered (GeoPolRisk).

5.5 Characterisation factors (excerpt, including qualitative and quantitative discussion of variability and uncertainty)

Table 5.3 presents an excerpt for a set of mineral elementary flows for the seven recommended LCIA methods [12].The selection includes those resources contributing more than 10% to impacts in the case study (Chapter 5.6).

5.6 Application to a case study

The impact assessment methods recommended in the first and second phase of the global guidance on LCIA indicators project were tested in a common case study on the LCA of cooked rice (Frischknecht et al. 2016). This case study comprises the cultivation, processing, distribution, and cooking of white rice and, thus, is very suitable for testing impact assessment methods for land and water use, climate change, or acidification and eutrophication, human and ecotoxicity. However, the life cycle inventory contains only a few mineral resources with low amounts. Given that mineral resources are the focus of this task force, the scope of the rice LCA case study was reduced from the entire life cycle to the transportation of rice from the grocery store to home. A transport distance of 1 km driven by means of an electric vehicle was assumed and an existing LCI (Stolz et al. 2016) that comprises the extraction and use of several mineral resources was used as a basis to apply the seven selected impact assessment methods.

Figure 5.3 displays the potential impacts of all the minerals included in the LCI of the EV life cycle

12 Complete list of Characterisation factors are available for download from: http://www.lifecycleinitiative.org/applying-LCA/LCIA-CF

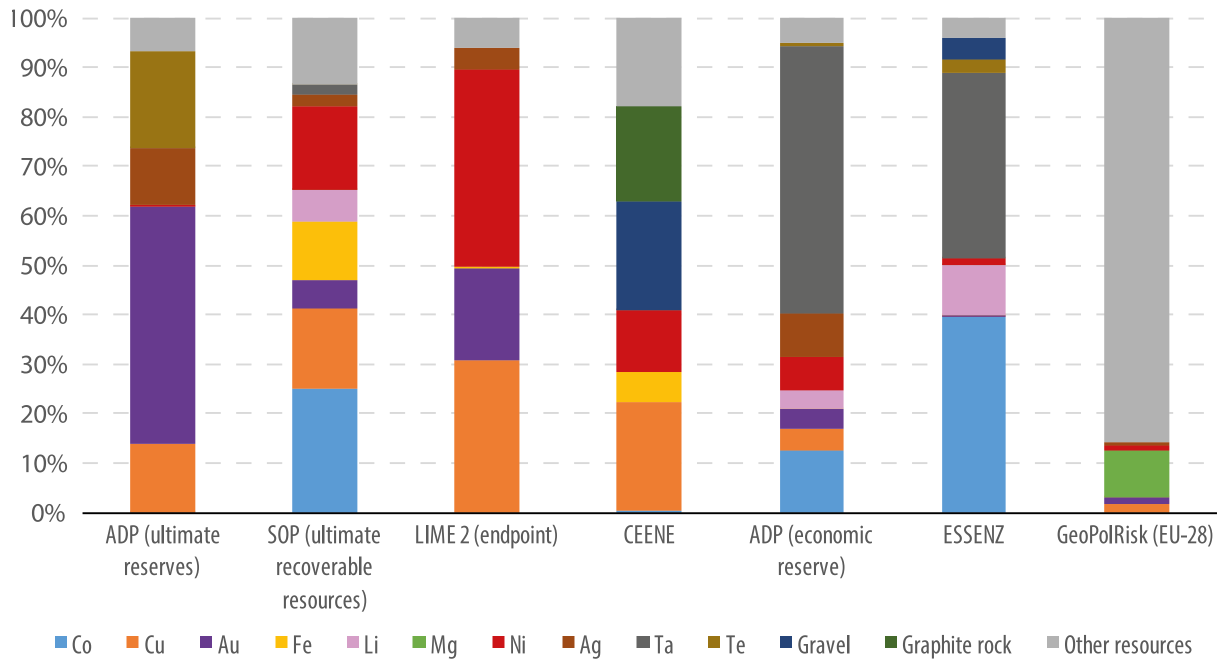

Figure 5.3. Case study impact assessment results for the selected methods (driving 1 km with an electric car)

(extraction of 34 primary mineral resource elements, 37 primary mineral resource aggregates, excluding energy carriers, Stolz et al. 2016). Only resources contributing more than 10% to at least one impact category are reported separately, while the others are grouped under the category "other resources." Since the number of CFs can differ between LCIA methods and cover different elementary flows, care should be taken when interpreting the LCIA results to not confuse a null with a missing CF.

Several observations can be made:

1. Gold dominates the result for $ADP_{\text{ultimate reserves}}$ due to its relatively low abundance in the earth's crust. In contrast, tantalum dominates the result of $ADP_{\text{economic reserves}}$ implying that these current economic reserves are under relatively high pressure due to current extraction rates, which can be considered as a mid-term physico-economic availability constraint. The different results in the two ADP versions reveal the strong influence of the respective natural stock (ultimate vs. economic reserves) in the characterisation model (see equation 1 in 5.4).

2. Copper causes a relevant contribution in all of the inside-out related methods (13-31%) but in none of the outside-in focused methods (<5%).

3. Besides copper, nickel is another large contributor to the result for the future efforts methods (SOP and LIME2) and for the CEENE method.

4. Cobalt causes a relevant contribution in outside-in methods ($ADP_{\text{economic reserves}}$ and ESSENZ) as well as in one of the inside-out methods (SOP).

5. Cobalt and tantalum are the main contributors to the result for $ADP_{\text{economic reserves}}$ and ESSENZ (the GeoPolRisk method does not have CFs for these minerals).

Even though GeoPolRisk and ESSENZ address short-term geopolitical, socio-economic supply risks, the results differ strongly. This can be explained by the different supply risk aspects considered and by the perspective on global production (ESSENZ) or European imports (GeoPolRisk). A comprehensive discussion of the case study results obtained by the supply risk methods are published by the members of the supply risk subgroup (Cimprich et al. 2019)

Even though we focus on LCIA methods, keep in mind that there are some resource-specific LCI challenges that heavily influence the LCIA result. For instance, allocation of metals in multi-metal ores is accomplished in mainly two different ways by LCA practitioners and database providers: either the metal content of the ores entering the product system is allocated to the produced metals based on physical mass balances and the remaining inputs and outputs based on economic or other relationships (as for this case study), or the ore in its entirety (containing different metals and gangue) is allocated to the products using economic relationships. These two allocation procedures are comprehensively discussed in Berger et al. (2019) but no recommendation for one way or the other could be agreed upon within this task force.

5.7 Conclusions and outlook

There are many types of questions in terms of resource use in product systems that LCIA methods users would like to answer. In this work, a safeguard subject for mineral resources has been defined and major questions on the impacts of mineral resource use were categorised into two general categories of impacts that occur, either inside-out (changing opportunities for future generations to use resources due to current resource use) or outside-in (potential resource availability issues for a product system). The two major questions have been specified into seven more specific questions and existing impact assessment methods have been recommended to answer them (see Table 5.1). For all the recommended methods, there are still some aspects that could be added or be improved. These improvements are discussed in the following, starting with some general recommendations.

5.7.1 Recommendations for method improvement and development

Some general recommendations apply to many (or all) methods: CFs need to be regularly updated. The aim should be to increase the number of elementary flows with more robust CFs, and uncertainties should be addressed. Furthermore, except for AADP, none of the existing methods considers anthropogenic stocks, whereas the agreed upon safeguard subject includes them. Therefore, this is an opportunity of improvement across all method categories. With regard to implementation of CFs, method developers should coordinate with software developers to make sure that new or updated methods are incorporated in newer versions of LCA software.

Depletion methods

It is recommended to consider the full extraction rather than the currently used net production, which neglects flows of material ending up in tailings, waste rock, or as emissions to nature. Considering the relevance of the anthropogenic stock and "dissipative resource use" (see Section 5.7.2) as the actual reason for the depletion of total stocks (natural + anthropogenic), the characterisation models of depletion methods could be adopted to reflect the dissipation of total stocks.

Future efforts methods

SOP method – It is recommended that CFs be empirically derived for a greater number of resources to reduce the uncertainty of SOP CFs. Additionally, there is lower confidence in the method's underlying assumption of preferential extraction of higher-grade ores for by-product and co-produced resources, as the extraction of these resources are heavily influenced by the extraction of the primary 'host-mineral.' Further work to establish the strength of correlations between co- or by-produced resource grades and host-mineral grades may provide more confidence in the assumptions underlying the SOP method.

Ore grade-based methods – Ore grade is only one relevant measure of resource quality that influences resource extraction, with other measures including aspects such as resource accessibility (e.g., depth, morphology, and location) and mineral complexity (e.g., mineralogy, particle size distribution and grain 'texture'). These other aspects of resource quality are not considered in detail by existing methods. As mining costs and mined ore grades are heavily influenced by short-term trends in market conditions, ensuring that the characterisation factors are reflective of relative rates of declining resource quality would require that the short-term influences of commodity prices be controlled. This is particularly relevant to the ORI and SCP methods that develop characterisation factors directly from mining industry data for particular time periods. Therefore, the development of characterisation factors using baseline ore grade and cost data over multiple commodity price cycles is required before these or similar methods could be recommended.

Economic externalities – LIME2 and the future welfare loss method apply different approaches to assess economic externalities with regard to future users. In environmental economics, there are other approaches that mainly focus on economic externalities for the current generation. These different temporal perspectives might be discussed and reflected in future method developments.

Thermodynamic accounting methods

New approaches for metals and minerals could be developed, for instance by creating new reference states that better reflect their societal values. The choice for a reference state ought to differ according to different problem-definitions. Thermodynamic accounting methods can be used to assess a broad range of resources including fossil energy carriers, land, wind (kinetic) energy, hydropower (potential) energy, and water, among others.

Supply risk methods

Future method development should consider geopolitical and socio-economic availability constraints of secondary resources and intermediate products, which also can pose a supply risk for companies. Moreover, it is recommended to validate and refine characterisation models using empirical evidence of supply risks. Instead of considering the import structure of countries, it is suggested to consider the specific purchase structure and supply chains of companies.

5.7.2 Outlook on dissipation

The main discussion point with regard to further method development was the inclusion of the dissipation concept. The discussion of resource dissipation starts from the fact that mineral resources are not lost for human use when extracted into the technosphere as long as they can be reused, recycled, or restored. They are only lost if brought into an irrecoverable state, which might be called a dilution loss (van Oers et al. 2002) or a dissipative loss (Stewart and Weidema 2005). Following this basic concept implies that a) the inventories need to be complemented with information about dissipative losses instead of resource extraction only and b) the impact assessment methods should also take into account dissipation rates instead of extraction rates, as well as the total stock, i.e., the natural and the anthropogenic stocks. To date, neither one nor the other has been implemented. However, some suggestions exist on how to deal with dissipation on both levels:

LCI – Given the current lack of data in inventories, Frischknecht and Büsser Knöpfel (2013) and Frischknecht (2014) suggest an inventory correction, crediting recycled resources, in order to capture dissipative use because they suggest applying existing impact factors on the dissipative use of resources. Zampori and Sala (2017) describe different alternatives on how to structure Life Cycle Inventories to capture dissipation and provide simplified cases studies to evaluate the features of a dissipation approach.

LCIA – van Oers et al. (2002) and van Oers and Guinée (2016) discuss how the ADP equation could be adjusted for inclusion of dissipation or in their terms "dilution" of resources. If the extraction rate in the equation (E in equation 1) is replaced by the dissipation rate, or in their terms "leakage" (the dissipation from technosphere to environment). This should then be combined "with the total reserve of resources in the environment and the economy," i.e., the total of the natural and the anthropogenic stocks (instead of R in equation 1).

In order to make the dissipation concept applicable in LCA, the following issues need to be resolved:

The dissipation threshold – The threshold between dissipative and non-dissipative resource use is not an absolute one but depends on technological and economic factors, which can change over time. Furthermore, a definition of resource quality might be needed to be able to set the quality threshold beyond which a quality loss is considered to be a dissipative loss. Resource quality information such as concentration also needs to be integrated in resource inputs and outputs in life cycle inventories.

Dissipation within the technosphere – Dissipation into the ecosphere (the environment) happens for example by dispersion into irrecoverable concentrations in environmental compartments (air, water, and soil), whereas dissipation within the technosphere may include for example using minerals in alloys, which may in some cases make a separation of the alloying elements "essentially impossible" (Reck and Graedel 2012), or the unwanted mixing of metals in recycling processes, or low absolute amounts of resources in landfills making extraction unprofitable regardless of the concentration.

In both cases, dissipation into the ecosphere and dissipation within the technosphere, the dissipation implies that for the use of another unit of the resource, additional resources will need to be extracted either from the environment or from anthropogenic stocks.

The issue of occupation or borrowing – Another issue with regard to a "loss" within the technosphere is the issue of resource occupation or "borrowing" (van Oers et al. 2002; Frischknecht 2016): As long as resources are in use, they are not available for other users although they might not be dissipated (yet). This constraint to resources availability is not directly addressed by the dissipation concept (other constraints may similarly be missed, e.g., geopolitical constraints). It is debatable whether resource occupation beyond a maximum lifetime should be assessed as if it was dissipative use as suggested by Frischknecht (2016).

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6. Land Use Impacts on Soil Quality

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6.1. Scope

Soils are the loose upper layer of the Earth's surface, composed of '*weathered mineral materials, organic material, air and water*' (FAO 2018). According to a common definition from soil scientists, *"soil quality is the fitness of a specific kind of soil to function within its surroundings, support plant and animal productivity, maintain or enhance water and air quality, and support human health and habitation"* (Karlen, Mausbach et al. 1997). This definition emphasises both inherent properties of soil ("*a specific kind of soil*") and dynamic interactive processes (Larson and Pierce 1991), and links soil quality to its functions, which contribute to ecosystem services.

Soils contribute to ecosystem services including: i) provisioning (e.g., fresh water), ii) regulating (e.g., climate regulation), iii) cultural (e.g., recreation) and iv) supporting services (e.g., primary production) (World Resources Institute 2005; Dominati, Patterson et al. 2010; Adhikari and Hartemink 2016; Cowie, Orr et al. 2018). The central role of soils for ecosystem services justifies that they are addressed specifically across several Sustainable Development Goals (SDGs), including 2.4 (sustainable food production systems) and 15.3 (striving to achieve a land degradation-neutral world). Due to the complex spatial and temporal characterisation of soil functions and properties across multiple Earth's spheres (lithosphere, biosphere, atmosphere, hydrosphere) and scales, modelling of soil processes and their associated services is a challenging task (Adhikari and Hartemink 2016).

Soil functions are determined by pedoclimatic variables such as soil texture, soil organic matter, rainfall, temperature, and related biological parameters. Assessing the effects of human interventions on soil quality requires a geographic scale that is sensitive to these variables and is relative to the optimum soil quality possible within a given context.

Land use and land use change (LULUC) are key human stressors that affect soil quality, e.g., by modifying physical, chemical, and biological properties of soil through agriculture and forestry, by altering the rate of removal of soil, and/or sealing it through infrastructure. Other significant impacts on soil quality can be caused by the presence and/or accumulation of contaminants in soil, leading to acidification or toxic impacts. The potential impacts of human interventions on soil quality through LULUC and the associated management practices make the inclusion of a soil quality indicator essential for many life cycle assessment (LCA) studies of product systems that transform or occupy land. This chapter focuses exclusively on the impacts from LULUC on soil quality and does not address toxicity or eutrophication, which are dealt with in other chapters.

6.2. Review of approaches and indicators

This section reviews existing life cycle impact assessment (LCIA) methods with available characterisation factors that are relevant for soil quality and that were considered for recommendation. Current LCIA models do not provide a harmonised comprehensive assessment of soil quality. They focus on various indicators covering various physical, chemical, and biological properties. The most common models address soil organic carbon, soil erosion, and biological productivity. Only one model, the land use indicator value calculation in life cycle assessment (LANCA®) model (Bos, Horn et al. 2016), combining several approaches, also includes groundwater regeneration, mechanical filtration, and water infiltration capacity. We detail hereafter the first three most-encountered indicators. A more comprehensive description of the methods and models is given by Vidal Legaz, Maia De Souza et al. (2017), including key methodological elements and original sources.

6.2.1 Soil organic carbon

Change in soil organic carbon (SOC), usually in kgC/m^2, has been proposed to be used in LCIA by several authors (Mattsson, Cederberg et al. 1990; Cowell 1998; Baitz, Kreißig et al. 1999; Milà i Canals and Polo 2003; Milà i Canals, Romanya et al. 2007; Brandão and Milà i Canals 2013) as a good indicator for soil quality. It is causally associated with other important indicators including: soil fertility and biotic production; carbon and nutrient cycling; and water infiltration and erosion protection (see Figure 6.1). The ultimate effects of SOC change on final ecosystem services (e.g., those delivered to ultimate human beneficiaries) require further modelling to consider the change in biotic production and the fraction of this biotic production that provides benefits to humans (e.g., climate change mitigation, provision of biomass for food, fibre, and feed).

The change in SOC is measured relative to a reference state which Brandão and Milà i Canals (2013) term potential natural vegetation (PNV). The SOC values have broad global coverage and are geographically differentiated based on climate regions. As for the coverage of land and management practices, Brandão and Milà i Canals (2013) include different SOC characterisation factors values for land use intensity (low input, medium input, high input without manure, high input with manure) and tillage practice (full tillage, reduced tillage, no tillage) based on the parameters used in the Intergovernmental Panel on Climate Change (IPCC) calculations for total soil carbon change.

6.2.2 Biomass production

Biomass production is correlated to a change in SOC, itself influenced by the combination of other factors including soil type, climate region, land cover, and management practices. Indeed, SOC reflects the balance between inputs of organic matter derived from biotic production and the turnover related to soil biological activities. Hence, changes in biotic production leads to a new equilibrium SOC level. As soil quality determines productive potential, and therefore biomass production, change in biomass production as indicated by change in SOC is relevant to soil quality.

Impact on biomass production is proposed in a number of LCIA models (Núñez, Antón et al. 2013; Alvarenga, Erb et al. 2015; Bos, Horn et al. 2016), although different indicators and pathways are considered in each model. Net primary production depletion (NPPD) was proposed by Núñez, Antón et al. (2013) in which soil loss through erosion is linked to a loss of biomass production (as well as damage to natural resources). Human appropriation of NPP (HANPP) was proposed by Alvarenga, Erb et al. (2015), which measures the NPP consumed by humans and, therefore, not available for ecosystems, by looking at the difference between NPP of potential natural vegetation and the current land use. Biotic production loss potential (BPLP) proposed by Bos, Horn et al. (2016) is obtained by the difference in biomass production between the current and the reference land use. Where a PNV reference state is used for BPLP it would represent the same outcome as HANPP, with both measuring the difference in biomass production between the modified land use and a PNV baseline.

In Núñez et al. (2013) and in Bos, Horn et al. (2016) the value of NPP is dependent on climate, soil properties, and the sealing factor.

6.2.3 Erosion

Erosion can be modelled in LCIA as a result of LULUC as is done by Bos, Horn et al. (2016) but there are methods that add erosion as a life cycle inventory (LCI) elementary flow, as is done by Núñez, Antón et al. (2013). In both of these methods, water erosion potential is calculated using the revised universal soil loss equation (RUSLE) (Renard, Foster et al. 1991), which depends on soil characteristics, rainfall, slope, land cover, and management activities (Bos, Horn et al. 2016). In this report the LCIA pathway is examined as it is better suited to existing LCI datasets.

6.2.4 Other impact categories

In addition to the indicators presented above (SOC, biotic production, and erosion), models have also been proposed for groundwater regeneration, water infiltration capacity, and physicochemical filtration reduction.

Bos et al. (2016) describes how different types of land use can contribute to soil sealing, which can affect surface water flow and evapotranspiration, and subsequently the rate of groundwater regeneration.

Bos et al. (2016) is the only LCIA model that accounts for the impact of soil sealing on water infiltration capacity. Infiltration reduction potential (IRP), an indicator representing a loss of soil mechanical filtration capacity, is affected by soil characterised permeability [cm/(d*m^2)], which depends on soil, land use type, distribution of pores, and depth to groundwater table (Beck, Bos et al. 2010; Bos, Horn et al. 2016).

Soil regulates water flow and the transport and storage of other substances that can affect water quality. Changes in organic matter affect its capacity to store substances such as nitrogen compounds that can affect water quality. Bos, Horn et al. (2016) use cation exchange capacity (CEC) as the corresponding impact indicator. Soil organic matter, of which SOC is the major component, accounts for the largest share of CEC in mineral soils (50-90%) and is thus a key indicator for the filtration and buffering capacities of soils (Brady and Weil 1999).

6.2.5 Summary of approaches and indicators

In conclusion, there are currently a limited number of LCIA models covering a number of impact pathways addressing soil quality issues. However, there is still no comprehensive approach to soil quality assessment. Soil processes are complex, and the impacts of LU are wide-ranging. More research work is needed in order to develop a model assessing, if not all indicators, at least a comprehensive set of soil quality-mediated impacts of LU on ecosystem services and other damage categories. New models are also needed for connecting the impacts from land use occupation and transformation to the damages endpoints defined by Verones, Henderson et al. (2016). Moreover, only a few of these models allow for deriving characterisation factors with both global coverage and regionally specific declinations.

6.2.6 Reference states

Since evaluating the environmental effects of land use is always in comparison to a reference situation, this land use reference state needs to be clearly defined. Saad, Koellner et al. (2013) propose the use of potential natural vegetation (PNV) at the scale of terrestrial ecoregions based on Olson *et al.* (2001) as the reference state. Bos, Horn et al. (2016) defined their reference as the largest natural biome (in terms of surface area) in each country, but this created anomalies especially in countries with large low-productivity land or land not managed for agricultural or forest production such as Australia, with desert being the reference state. In an update to the factors in 2019, the reference state was calculated as a weighted average of the values of ecosystem quality for all the types of PNV that can be found in a country according to the global map of ecological zones provided by FAO (2012). The weighted average was calculated considering the area share of each ecological zones in a country and excluding, for agricultural and forest-related land use types, the following ecological zones: "boreal tundra woodland," "polar," "subtropical desert," "temperate desert," and "tropical desert" (De Laurentiis, Secchi et al. 2019). Although Saad et al. (2013) also used the framework developed in the LANCA model, they propose that the reference state be based on PNV using Holdridge life zone level (Holdridge, 1947 #2047) (a combination of climatic conditions and vegetation cover that provides simpler classification–only 38 life zones globally, compared with 867 ecoregions). This potentially provides a more comparable baseline than used in LANCA and is consistent with the baseline chosen for the biodiversity model provisionally recommended for land use impacts on biodiversity at the last Pellston Workshop (Chaudhary, Verones et al. 2015), which was the natural or close to natural vegetation habitat per ecoregion (Frischknecht and Jolliet 2016).

6.3. Process and criteria applied and process to select the indicator(s)

For the purpose of incorporating soil quality impacts within LCA, ideally the choice of the indicators should comply with the following criteria:

- Soil quality should be represented by a minimum number of indicators, in order to avoid the multiplication of recommended indicators, with causal links to the main soil functions to enable efficient interpretation of impacts;
- The indicator should be compatible with existing land use LCI flows, i.e., related to land occupation and transformation elementary flows, but may also recommend additional elementary flows;
- The indicator should be applicable globally, to all types of land use, for both background and foreground processes.

One approach to derive a metric for soil quality is through a soil quality index (SQI).

The Swiss agricultural life cycle assessment (SALCA) model (Nemecek, von Richthofen et al. 2008) combines several indicators using a mechanistic process-based composite model into an SQI, but was not considered for inclusion in this assessment, as it was developed specifically for the Swiss context and relies mostly on expert knowledge and detailed primary data. The detailed data requirements make this model incompatible with the global scope of LCIA.

A type of SQI was developed by the European Commission's Joint Research Centre (JRC) that included aggregating four of five indicators from the LANCA model (Bos, Horn et al. 2016). However, the weighting system was viewed as subjective, as all indicators were given the same weighting in the index. As physicochemical filtration and mechanical filtration indicators presented a unitary correlation coefficient, only the latter was included in the aggregation to avoid accounting for potentially redundant information (De Laurentiis, Secchi et al. 2019).

Several authors agreed that a contribution based on observed correlations using multi-parametric statistics could be used to link soil quality attributes to a one-dimensional SQI (Andrews, Karlen et al. 2002; Velásquez, Lavelle et al. 2007; Obriot, Stauffer et al. 2016). However, such an approach is not currently available, and failing this, there is no consensus on alternative approaches to calculate a soil quality index (Andrews, Karlen et al. 2004; de Paul Obade and Lal 2016; Obriot, Stauffer et al. 2016).

Given the limitations of existing LCIA models described above, soil organic carbon (SOC) remains the only available indicator that is both comprehensively linked to several soil quality functions and is applicable within the LCIA framework. SOC is a soil property that mediates many cause-effect links between soil properties and soil functioning (Dominati, Patterson et al. 2010; Cowie, Orr et al. 2018). In particular, SOC is to some extent an implicit indicator of the amount of soil biota present in soil. SOC is positively correlated with the four key soil functions as defined by Kibblewhite, Ritz et al. (2008): carbon transformations; nutrient cycling; soil structure maintenance; and the biological population regulation of soil fauna. As summarised by FAO[13] "SOC transcends all chemical, physical, and biological soil indicators and has the most widely recognized influence on soil quality as it is linked to all soil functions." We hence recommend using change in SOC, in kg C, as a midpoint indicator for soil quality impacts from LULUC.

It is recognised that SOC does not represent all aspects of soil quality. Erosion, chemical pollution and salinization are processes that have a weak correlation with SOC (Milà i Canals and Polo 2003; Milà i Canals, Romanya et al. 2007). Since soil loss is considered a critical soil threat (Yang, Kanae et al. 2003), we also therefore recommend quantifying soil loss from erosion using the LANCA model (Bos, Horn et al. 2016), initially as a midpoint, but ultimately with a view to include it within the socio-economic assets damage category. Chemical pollution of soils is covered through ecotoxicity and acidification indicators, while salinization is not currently considered.

6.4. Description of the impact pathway and indicators selected

Figure 6.1 presents the impact pathway linking LULUC to the damage categories via processes that impact soil properties, soil functioning, and ecosystem services. The life cycle inventory is based on land occupation and land transformation under different types of land cover and land management. These occupations and transformations can include processes (e.g., sealing, compaction, etc.) that have direct impacts on soil properties (e.g., SOC content, soil structure, soil

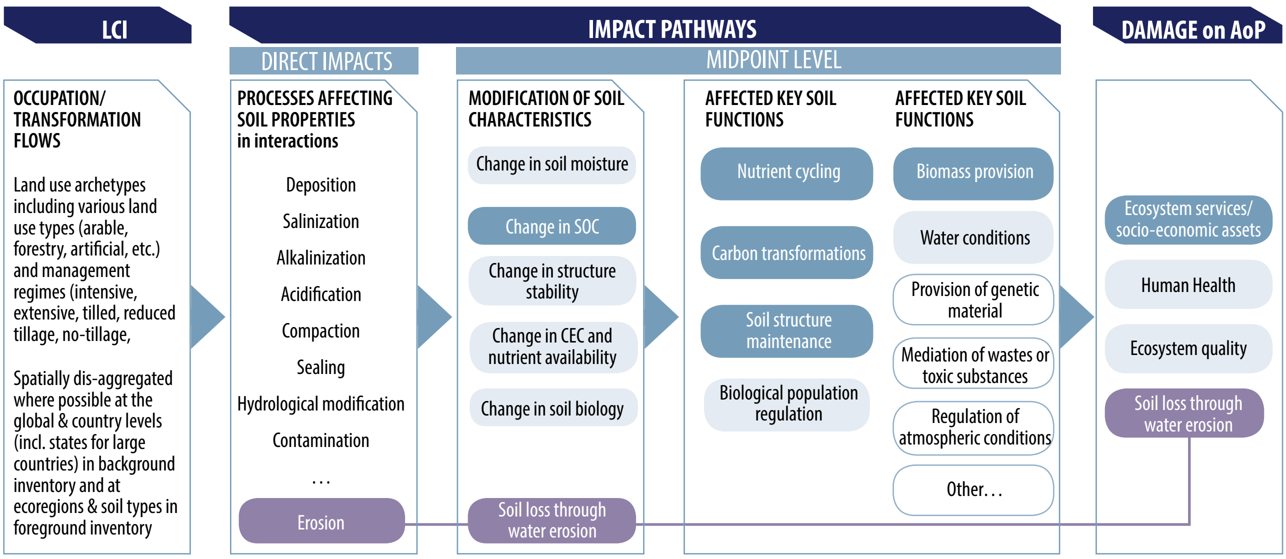

Figure 6.1. Impact pathway of land use impact on soil quality and soil loss through water erosion

13 http://www.fao.org/soils-portal/soil-degradation-restoration/global-soil-health-indicators-and-assessment/en/

moisture) and can affect soil functions (e.g., nutrient cycling) and the ability of soils to provide ecosystem services (e.g., biomass provision).

Figure 6.1 shows the two selected indicators with the cells highlighted in dark blue being the impact pathway for change in SOC and cells highlighted in red is the pathway for soil loss through water erosion. While three soil functions are identified in the change in SOC pathway, many soil functions and ecosystem services are connected and are shown in lighter shades of blue to represent softer links to the SOC pathway. Similarly, for erosion the impact pathway is connected to natural resources but may also have links to other damage categories such as socio-economic assets. For simplicity, we present just a few key ecosystem services from the Common International Classification of Ecosystem Services (CICES)[14]. Additional ecosystem services may be affected by other changes in soil quality due to LULUC that are not captured in this figure.

6.5. Model, method and specific issues addressed

6.5.1 Calculation of land occupation and transformation impacts

The two types of land use interventions as described by Koellner, De Baan et al. (2013) are land transformation and land occupation. In the context of our soil quality indicators, land occupation is quantified by the area of land and the time for which it is occupied in units of m²•year. The impact of occupation is the difference between the quality of the land in the occupied state and the reference state as shown in Equation 1. The reference state in the selected methods is potential natural vegetation.

Equation 1

$$\text{Occupation impact} = (A_{FU} * t_{FU}) * (Q_{Ref} - Q_{LU})$$

Where Occupation impact is in kg SOC deficit•year or kg soil lost

A_{FU} is the area of the functional unit in m²,

t_{FU} is the time of occupation for the functional unit in years,

Q_{Ref} is the quality of the land in the reference state in kg C or kg soil loss/ year, and

Q_{LU} is the quality of the land in the occupied state in kg C or kg soil loss/ year.

Transformation is measured in m² as the act of transformation is taken to occur over a short period and in LCA is assumed to be instantaneous. Physical damage to land during the process of transformation is not quantified in LCA[15]. What is quantified are the impacts of occupying the land during the time it takes to return it to the quality under the prior land use, with the time taken referred to as the regeneration time. Transformation effects are calculated as the difference in land quality multiplied by half the regeneration time as shown in Equation 2.

Equation 2

$$\text{Transformation impact} = A_{FU} * (Q_{LU2} - Q_{LU1}) * t_{reg} / 2$$

Where Transformation impact is in kg SOC deficit•year or kg soil lost

A_{FU} is the area of land transformation in m²,

Q_{LU2} is the quality of the land after transformation in kg C or kg soil loss/year,

Q_{LU1} is the quality of land prior to transformation kg C or kg soil loss/year, and

t_{reg} is the regeneration time to achieve the quality of the prior land use in years.

Life cycle inventories generally include paired flows for "land transformation from," and "land transformation to" so the quality change is measured from the reference state. However, when the two are combined the reference state cancels out of the equation.

6.5.2 Soil organic carbon (SOC) deficit potential

SOC deficit potential has been defined as the change in soil organic carbon (ΔSOC) over a period of time relative to a PNV reference state. ΔSOC is recommended as a midpoint impact indicator with further investigation required to link this to related damage category.

We retain the model presented by Brandão and Milà i Canals (2013) for calculating characterisation factors (CFs) for SOC deficit potential. The proposed CFs for land occupation are defined as the ΔSOC between the reference land use and the current land use over

14 https://cices.eu/cices-structure/

15 For example, when clearing natural vegetation for use as cropping land the erosion from tree removal prior to establishment of the crop is typically not quantified.

the occupation time (kg C * m $^{-2}$). Multiplying the land occupation CF by the land occupation inventory flow (m^2 • year) results in a ΔSOC in units of kg C • year, which represents the time integrated ΔSOC between the reference land use and the current land use (SOC deficit potential).

Characterisation factors for land transformation represent the time-integrated ΔSOC during the regeneration time between the previous land use and the new land use in kg SOC (kg SOC * m^{-2} * yr). Multiplying the transformation characterisation factor by the inventory flow for land transformation (m^2) results in a transformation impact of ΔSOC in units of kg SOC•year (SOC deficit potential). Only national average characterisation factors have been developed based on potential natural vegetation as the reference land use.

CFs proposed in Brandão & Milà i Canals (2013) are based on default SOC data for climate regions and soil types and under different land use and management conditions reported by the IPCC (Eggleston et al. 2006). These IPCC estimates are based on soil data from the National Soil Characterization Database (USDA 1994), the World Inventory of Soil Emission Potential Database (International Soil Reference and Information Centre), and data on SOC compiled by (Bernoux, da Conceição Santana Carvalho et al. 2002). For the purpose of greenhouse gas (GHG) accounting, IPCC 'default data' is applicable to the simplified tier 1 accounting methods, whereas tier 2 and tier 3 approaches are recommended when more specific data are available. These more detailed approaches could be used to improve the SOC deficit model.

6.5.3 Erosion potential

Soil erosion induced by movement of water is estimated using the revised universal soil loss equation (RUSLE), based on the approach by Bos et al. (2016) with revisions (Horn and Maier 2018) to the reference state mentioned in Section 6.2.6 and the inclusion of regeneration times for land transformations from Brandão and Milà i Canals (2013). These regeneration times were added for compatibility with the approach in the SOC deficit potential indicator and LCIA of land use approach recommended by UNEP-SETAC (Koellner, De Baan et al. 2013). Characterisation factors for soil erosion from water include land occupation effects in kg soil m^{-2} $year^{-1}$ and land transformation in kg soil m^{-2}. Multiplying the occupation and transformation characterisation factors by the inventory flow for land occupation (m^2•year) and land transformation (m^2) results in a occupation and transformation impact in kg soil loss (erosion potential).

LANCA (Bos, Horn et al. 2016) also suggests to consider some land transformations with no possible regeneration as permanent transformation, which is not considered in the presented approach. To avoid leaving these transformations out of LCA, the regeneration time from the supplementary data set provided in Brandão & Milà i Canals (2013) of 85 years has been applied for transformation to completely denuded areas such as construction and mining sites.

6.6. Characterisation factors

6.6.1 SOC deficit potential

CFs for SOC deficit potential are available for nine land use types in ten climate region levels and for six soil types, plus one set for global-default values based on the weighted average of the ten climate regions. In addition, several intensities for several of the land use types are provided (namely four different intensities for each of full tillage, reduced tillage, and no tillage agricultural land; three levels of degradation and two intensities for grasslands).

As no country specific CFs were provided in Brandão & Milà i Canals (2013), the following procedure is applied to provide these CFs: for each country considered, the geographical distribution of climate types (Joint Research Centre 2018) in that country are used to calculate country-specific characterisation factors. Then country-specific CFs are calculated as an area-weighted average of the CFs provided for the different climate regions. When aggregating, only areas where a certain land use activity can take place are considered, excluding deserts and permanent snow-covered areas from the aggregation.

Table 6.1 shows the global factors from Brandão & Milà i Canals (2013), as well as derived factors for one country (China) using the climate regions calculation.

6.6.2 Erosion potential

For the quantification of erosion potential from land use activities, the set of characterisation factors proposed by Bos et al. (2016) are recommended

Table 6.1. Occupation and transformation CFs for soil organic carbon deficit potential (for global average and 1 country example [China]) for different land use types

Land use	Land use sub-category	World (occup.) tC.yr ha^{-1}yr^{-1}	China (occup.) tC.yr ha^{-1}yr^{-1}	World (trans.)	Transformation avg global
Long-term cultivated	Unspecified	21	16.0	205	160.0
Long-term cultivated full tillage	Unspecified	21	16.0	205	160.0
	Low input	23	18.7	231	187.4
	Medium input	21	16.0	205	160.0
	High input without manure	17	12.9	175	129.1
	High input with manure	5	-1.4	50	-13.8
Long-term cultivated Reduced tillage	Unspecified	18	13.8	176	138.2
	Low input	20	16.7	203	167.2
	Medium input	18	13.8	176	138.2
	High input without manure	14	10.5	142	105.3
	High input with manure	1	-4.5	8	-44.8
Long-term cultivated No tillage	Unspecified	15	10.6	148	105.5
	Low input	18	13.7	177	136.5
	Medium input	15	10.6	148	105.5
	High input without manure	11	7.0	112	70.4
	High input with manure	-3	-9.1	-31	-90.6
Permanent grassland	Permanent grassland	0	0.0	0	0.0
	Nominally managed (non-degraded)	0	0.0	0	0.0
	Moderately degraded	2	2.9	24	28.8
	Severely degraded	17	17.8	175	178.0
	Improved grassland - medium land management	0	0.0	0	0.0
	Improved grassland - high land management	-6	-6.5	-64	-65.2
Paddy rice		-6	-5.9	-58	-59.3
Perennial/Tree Crop		0	0.0	0	0.0
Set-aside (< 20 yrs)		8	7.4	80	73.6
Sealed Land		58	59.3	2465	2926.9
Forest		0	0	0	0

with the modifications to reference states discussed in Section 6.2.6, and inclusion of regeneration times discussed in Section 6.5.2, which have been implemented in the latest release (Horn and Maier 2018). CFs are provided by Bos et al. (2016) at both the global and country scale for a list of 58 land use types. A selection of the CFs calculated, based on the requirements of the rice case study to follow, are shown in Table 6.2.

6.6.3 Summary of proposed CFs

In summary, the new set of CFs was developed for both indicators. For the CFs for SOC, this was done by providing aggregated CFs at country level using climate data for each country and applying the climate-based CFs based on an areas weighted average.

The set of CFs to be used in the calculation of impacts on erosion potential were obtained by modifying the CFs provided in Horn and Maier (2018) and including the regeneration time in the calculation of transformation CFs.

In order to be consistent with the assumptions used in the calculation of the SOC CFs, regeneration times were taken from Brandão & Milà i Canals (2013) equal to 20 years for biotic land uses and 85 years for sealed land.

6.7. Rice case study application

A rice LCA case study was developed based on Frischknecht, Fantke et al. (2016) to illustrate the practical application of the proposed set of CFs and to identify needs for future development to improve their applicability in LCA. The case study includes three

Table 6.2. Selection of occupation and transformation CFs for erosion potential for global and 1 country example (China)

	World (occup.) kg soil $ha^{-1}yr^{-1}$	China (occup.) kg soil $ha^{-1}yr^{-1}$	World (trans.) kg soil ha^{-1}	China (trans.) kg soil ha^{-1}
Unspecified	-0.708	-1.060	-30.100	-45.200
Unspecified, natural	-0.661	-1.050	-6.610	-10.500
Forest, natural	-0.013	-0.005	-0.134	-0.052
Forest, secondary	0.007	0.001	0.072	0.013
Wetlands	-0.723	-1.070	-7.230	-10.700
Shrub land	-0.640	-1.040	-6.400	-10.400
Grassland/pasture/meadow	0.048	0.014	0.484	0.142
Grassland	0.048	0.014	0.484	0.142
Pasture/meadow, extensive	0.028	0.008	0.278	0.077
Agriculture	6.130	1.910	61.300	19.100
Arable	8.200	2.560	82.000	25.600
Arable, fallow	10.300	3.200	103.000	32.000
Arable, extensive	7.160	2.240	71.600	22.400
Arable, intensive	9.230	2.880	92.300	28.800
Arable, flooded crops	-0.034	-0.012	-0.341	-0.116
Arable, greenhouse	-0.040	-0.014	-0.403	-0.135
Permanent crops, extensive	7.160	2.240	71.600	22.400
Agriculture, mosaic	6.130	1.910	61.300	19.100
Urban	-0.708	-1.060	-30.100	-45.200
Industrial area	-0.712	-1.070	-30.300	-45.300
Construction site	13.700	3.440	583.000	146.000
Traffic area, rail/road embankment	-0.578	-1.020	-24.600	-43.500
Bare area	19.900	5.370	199.000	53.700

scenarios for rice production and use with one being rice grown in the U.S. and consumed in Switzerland, the second being rice grown and consumed in China, and the third being rice grown and consumed in India. Table 6.3 shows the inventory data for land occupation (m^2y) differentiated according to the land use classes used by Brandão & Milà i Canals (2013), and between foreground and background activities.

Table 6.3. Land occupation life cycle inventory results (cumulative land occupation) per land use classes [m^2y]

	USA - Switzerland	China	India
Annual crop (foreground)	1.40	1.46	2.69
Annual crop (background)	0.00	0.00	0.00
Perennial/tree crop (foreground)	0.00	0.00	0.46
Perennial/tree crop (background)	0.13	0.11	0.10
Sealed land (foreground)	0.01	0.01	0.00
Sealed land (background)	0.10	0.01	0.01
TOTAL	1.64	1.59	3.26

The CFs are provided aggregated at country level calculated from the original climate region CFs using areas of each climate type in each country. Information available in the rice case study was at the resolution of specific countries in which foreground activities would take place (i.e., the U.S., Switzerland, India, and China), and so country-specific characterisation factors were used for all foreground activities. The case study was also conducted using the global-default CFs, to assess how this would affect the results.

Case study results and discussion

Figure 6.2 shows the contribution analysis results for SOC deficit potential and erosion potential of the rice case study based on country-specific CFs for foreground activities. The agricultural phase (production) has the largest contribution for both indicators. For China, rice distribution also has noticeable impacts on SOC deficit potential. The SOC deficit potential from distribution is due to the high CF assigned to occupation as sealed land. Conversely, for erosion potential a negative impact (i.e., a benefit) is assigned to the distribution phase due to the negative CFs for occupation of artificial areas. Since the CF for

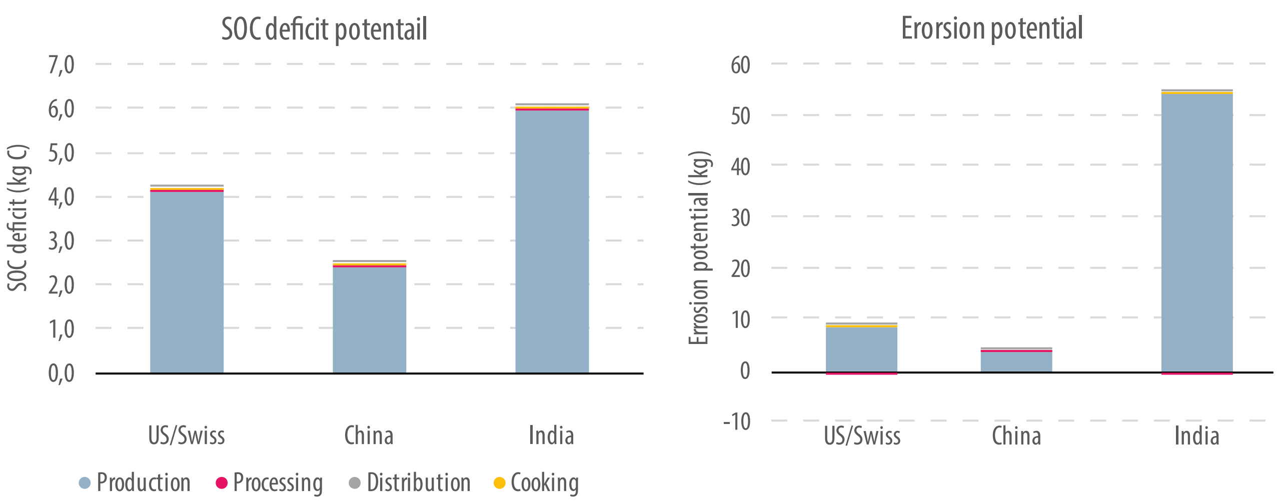

Figure 6.2. Contribution analysis for rice production: results for SOC deficit potential and erosion potential per kg rice cooked.

erosion potential is limited to water erosion, additional soil loss processes like wind erosion and soil removal for the purposes of construction activities are not included in this indicator. This concept is debatable, as sealing land represents a very invasive type of land use in terms of soil conservation, although it is less vulnerable to soil erosion from rainfall.

A comparison of the results obtained with country-specific and global-default CFs are provided in Figure 6.3. The higher impacts for India with the country-specific factor is directly related to higher inventory flows for land use for Indian rice production. For both impact indicators, the differences between the three options are less pronounced when using the global-default CFs. In particular, this can be seen in the case of erosion potential in India, which is more than double in the regionalised case compared with the non-regionalised case. This is due to the fact that the erosion potential CFs are higher for India compared with the global average due to rainfall intensity and topography. This highlights the importance of using country-specific CFs whenever the location of the activities being assessed is known.

6.8. Recommendations and outlook

The recommendations from the task force are broken up into specific recommendations for the choice of characterisation factors, judgement of the quality of these factors and the rationale for the level of recommendation. Further recommendations are then made on good practice for their implementation, inventory requirements, testing the CFs, and future developments.

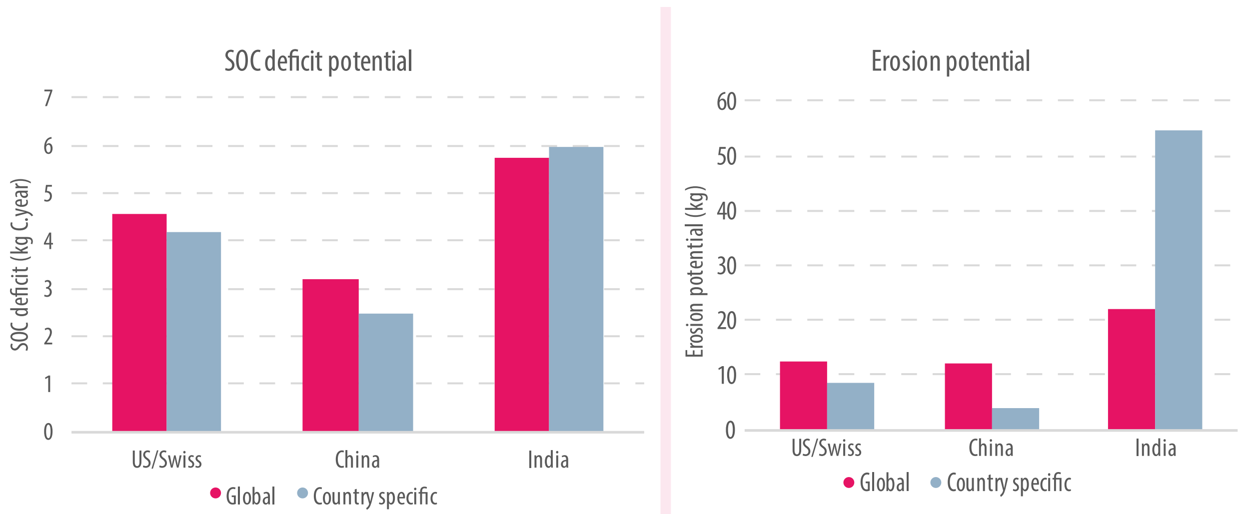

Figure 6.3. Rice case study results for SOC deficit potential and erosion potential using global and country-specific CF.

a) Main recommendations

- An interim recommendation (until necessary CFs are provided, see below) is to use SOC deficit potential based on Brandão & Milà i Canals (2013) with an expanded group of CFs for transformation and occupation of land use types including forests, grasslands, pastures, permanent crops, and artificial or sealed areas[16]. We recommend using CFs for SOC deficit with geographic resolution at the country or subnational (state, provincial, or regional) level where available. We strongly recommend basing CFs for SOC depletion potential on a spatial resolution that is relevant for the LULUC activity under study. For example, national production inventories should use national CFs, while local production may be based on ecoregion level CFs.
- In the absence of a complete model covering all forms of soil loss (wind erosion and water erosion including sheet, rill, gully erosion, and landslides), an interim recommendation is to use erosion potential based on RUSLE as proposed in Bos, Horn et al. (2016) with updates from Horn and Maier (2018), to model water erosion (sheet and rill erosion) after adjusting the reference state to PNV, calculating CFs at the ecoregion level and adding regeneration times for land transformation. These factors will be using regional (most likely national) characterisation factors to the extent permitted in the background LCA databases.
- We suggest that future work link erosion potential to the resource use endpoint accounting for soil dissipation through soil erosion and soil formation relative to the overall global soil resource, or potentially regional soil resources.
- We suggest linking SOC deficit potential indicator to biotic production potential and further to malnutrition and socio-economic assets consistent with approaches being implemented in water footprint links to human health and resources.

b) Judgement on quality, interim versus recommended status of the factors and recommendation

The reasoning for selecting the SOC deficit method is based on the maturity of the model as previously recommended by the ILCD in 2011 (EC JRC 2011) and because it has been used widely since then. SOC is a frequently cited indicator for soil quality that is strongly linked to the soil functions of carbon cycling, nutrient cycling, water retention and pest control, which link to endpoints including biotic production potential and other ecosystem services (Cowie, Orr et al. 2018). However, it is important to note that SOC deficit may be of limited value in areas where SOC is very high or where other important soil threats such as compaction or salinization exist, as increasing SOC in these areas may not enhance endpoints like biotic production and other ecosystem services. The recommendation for SOC deficit is provided as an interim recommendation until CFs are provided for major land use types such as intensive and extensive production forests and perennial crops, which are currently considered as having the same SOC as "natural forests."

Erosion potential is recommended as an additional indicator partly because SOC deficit potential does not have a strong link to the erosion of soil through water erosion. In addition, future work could link erosion potential to its impacts on socio-economic assets including costs for water quality treatment and dredging of reservoirs and rivers. However, in the absence of this link, we have an interim recommendation to use erosion potential as a midpoint indicator.

c) Applicability, maturity, and good practice for factors application

The SOC indicator is relatively mature with five years of use within the ILCD method. The changes proposed in this document are refinements rather than restructuring so the experience gained over this time remains relevant. The land management practices in the IPCC-derived factors (e.g., tillage with low - medium - high input, with and without manure, see Table 6.1) often have no direct correspondence in the elementary flows provided by Koellner, De Baan et al. (2013). It is recommended that users check whether information about tillage practices is available and such CFs may thus better represent the processes in their studied system.

For erosion potential, while the impact method was published in LANCA (2010), the underlying model (revised universal soil loss equation) dates back

16 Minority statement: the choice of SOC as a standalone proxy of soil quality implicitly results in a relevance of zero being given to soil qualities that are not or not well reflected by the SOC and this might not lead to an improved decision support as it risks neglecting relevant aspects.

to 1991 and its predecessor, the universal soil loss equation, dates back to 1965 (Wischmeier and Smith 1965) and is commonly used in soil sciences.

We recommend that both the SOC and erosion CFs are applied in background databases at the national level where the country is known or for states of large nations crossing multiple ecoregions, otherwise at the global level. In the foreground it is suggested that the specific soil type or the ecoregion level where the activity takes place is used where it can be calculated.

Special cases in organic soils (peatlands, organic wetlands): any transformation from these land covers are considered as a shift from the natural state, with the maximum impact. This is already considered in the CFs provided. Also, it should be noted that the ability of SOC to indicate soil quality in organic soils is limited (given that the SOC content is already very high, a slight increase or decrease would not be associated to a significant increase or decrease in quality in organic soils).

It is recommended to use the soil erosion potential in combination with the SOC deficit potential impact category because the indicators consider different impacts. For example, sealed land may reduce soil erosion but cause and increase in SOC deficit potential.

CO_2 emissions related to change in SOC influence climate change; the effects on climate change are not covered by this indicator, but those emissions may significantly affect the GHG emissions caused by the product system at issue. We strongly recommend that they are considered in the climate change impact category. Müller et al. (2012) provide an approach on this aspect.

d) Link to inventory databases (needs for additional inventory features, needs for additional inventory flows, classification or differentiation etc.)

For implementation of the factors in inventory databases most of the land use flows are already available in existing databases. New elementary flow names will be required with country names (and states for large countries) appended to the flow to encode the location until metadata with geolocations is supported in LCA software.

Geographic specificity is a common consideration in other impact categories such as water use and biodiversity impacts from land use activities. Other important flow data relevant for soil includes management practices such as tillage practices for different annual cropping. A correspondence table will be required to link the recommended characterisation factors to existing nomenclature. For example, the characterisation factor for an annual crop will link to all three flows: annual crop, annual crop irrigated, and annual crop non-irrigated.

e) Roadmap for additional tests

The SOC deficit model and erosion models are well understood, however, a number of refinements have been implemented including adjustments to the reference state and inclusion of regeneration times in erosion potential factors from Bos, Horn et al. (2016) and the calculation of country-specific factors for the SOC deficit model. The inclusion of these factors will be checked through a series of existing case studies in relevant production systems, including annual and perennial agriculture and forest products. However, the recommendations are not contingent on completion of these case studies.

f) Next foreseen steps

Adjustment to the characterisation factors needs to be implemented to ensure consistency with the land use elementary flows recommended by the Life Cycle Initiative (Koellner et al., 2013). The correspondence between land use elementary flows in Brandão & Milà i Canals (2013) and Koellner et al. (2013) will be based on the mapping exercise performed by the ILCD (Vidal et al 2017).

In 2019, it is expected that the IPCC will publish revised guidelines that include updated values management factors effecting SOC data, which should be examined for potential inclusion into the current method SOC method used in Brandão & Milà i Canals (2013).

A further development of the CFs provided for both indicators would be to provide them at a smaller geographical scale (e.g., states, ecoregions within a country, based on the coordinates). This would require that LCA software has the capacity to import geo-differentiated CFs, which is discussed in the cross-cutting issues chapter.

Following previous recommendations (Verones et al. 2016) there may also be a need for marginal characterisation factors where the reference land use is based on current land use activities. This option will require some investigation to determine if there is sufficient data to build a global set of characterisation factors, or if it may need to be implemented as part of the foreground of LCA studies.

As mentioned in Section 6.3, an integrative soil quality score could be an interesting option to explore to represent soil quality and its links to relevant endpoints. Kibblewhite, Ritz et al. (2008) highlighted the "*highly integrative pattern of interactions within each of the soil functions"* and proposed a new conception of soil quality based on the maintenance of its key functions. Such a model would be based on assessing directly the results of the soil functions (such as long term biotic production potential, water filtration, etc.) and not the factors involved in the underlying processes, such as SOC (Thoumazeau, Gay et al. 2018). The challenge in this work is to source data on soil quality that could be used to derive a predictive model of integrative soil quality, which is difficult on a global scale.

Calculation of default factors for global crops based on the global distribution of all crops can be undertaken in a similar way to the AWARE water footprint method which has agriculture and non-agriculture CFs (Section 5.5 in Frischknecht and Jolliet [2016]). Where crops grow is influenced by soil and climate conditions so aggregation of factors on a crop rather than geographic basis is both appropriate or feasible from a methodological point of view and practical in that it can be applied to the crop even when the location of the crop is not known. However, the use of CFs in background databases would be limited unless land use definitions include the name of the crop. Otherwise, the CF would be limited for use in the foreground of LCA studies.

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7. Ecotoxicity

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7.1 Scope

Chemical substances released into the environment are distributed across the various environmental compartments (e.g., air, water, soil) according to their physicochemical substance properties and the compartment characteristics. The potential of a chemical substance to cause harm (damage) to ecosystems (i.e., ecotoxicity potential) depends on its intrinsic properties (e.g., potency to induce an ecotoxicological effect), the characteristics of organisms, and the amount of time- and space-integrated exposure (which determines the effective exposure concentration) of the organisms in that compartment to the specific chemical. The concentration of certain chemicals has been shown to cause ecotoxicological impacts in various environmental compartments, with the extent of the impacts depending on the ambient concentrations, the mode of action and the sensitivity of individual species and the communities present (Schwarzenbach et al. 2006). The need to assure the safety of the use and disposal of chemicals into the environment has led to various treaties and regulations both for certain chemicals of concern as well as for the management of chemicals in general (e.g., Stockholm convention on persistent organic pollutants [ONU 2009] or the European Union regulation for the Registration, Evaluation, Authorisation and Restriction of Chemicals [REACH] [European Commission 2006]).

Ecotoxicity is one of the impact categories covered in environmental life cycle assessment (LCA) (Rosenbaum et al. 2018). Translation of the sum of all environmental emissions of chemicals associated with the production, use, and end-of-life of a good or a service into a measure of their potential ecotoxicological impacts is carried out in the life cycle impact assessment (LCIA) phase of LCA, using substance-specific characterisation factors (CF). These CFs should be derived from scientifically peer reviewed and accepted environmental models, which are adopted to operate within the restrictions posed by the boundary conditions of LCA (Hauschild and Huijbregts 2015). Because the number of chemical substances associated with the life cycle of a good or service can be large (tens to hundreds), the potential ecotoxicological impacts associated with a good or service life cycle are quantified for all relevant substances for which results are available in the life cycle emission inventory analysis of LCA. In the inventory, the emissions of each substance is scaled to the functional unit that the product or service system delivers. The location and time of the various emissions associated with a given product or service life cycle are often not known to an LCA practitioner, and their consideration in LCIA modelling software is not straightforward. Characterisation models currently used in LCIA are based on average situations and are sufficient to rank chemicals according to their toxicity potential for application in LCA whenever specific emission locations are not known. In contrast to ecological risk assessment, where conservative estimates are usually used to ensure safety, LCIA aims to reflect the average or most representative situations when comparing chemical substances with respect to their potential to cause harm and damage ecosystems (Hauschild and Huijbregts 2015).

There are many different potential impacts that could be considered when evaluating ecotoxicity, such as impacts caused by secondary poisoning (food web), impacts induced by specific modes of action, such as endocrine disruption, or effects on specific species. To express damage on ecosystems, the work of the Life Cycle Initiative and the approaches discussed in the present chapter use the potentially disappeared fraction (PDF) of species, a biodiversity-related metric for expressing damages on ecosystem quality (Curran et al. 2011).

Using the PDF as a metric to evaluate ecotoxicity enables comparison with potential impacts similarly resulting from other stressors in the life cycle inventory (e.g., acidifying substances or use of land), where damage (e.g., change in species biodiversity) is also expressed using PDF as a metric.

Various approaches have been developed to assess the potential impacts of chemical substances on ecosystems in LCIA (Hauschild et al. 2008b). Due to different assumptions and algorithms in these models, they lead to different results – different output metrics and scale-differences, of which numerical outcomes range up to a few orders of magnitude. To overcome intrinsic differences of the models and capitalise on the available knowledge, a global consensus model – USEtox – was conceived (UNEP-SETAC scientific consensus model for human and ecotoxicity characterisation modelling) (Hauschild et al. 2008a; Rosenbaum et al. 2008). USEtox enables the assessment of the potential impacts of chemicals emitted from product systems on ecosystems and human health. USEtox, as a consensus model, aims to represent mature science, while being open to incorporate new developments in scientific consensus as it evolves. For example, in the first version of USEtox, consideration of effects in coastal seawater and the soil compartment were excluded because the science was not considered mature or stable enough for a consensus model. Consensual recommendations from the ETF will be tested and evaluated in practical case studies and all underlying methods published – based on this, the recommended approaches will be suggested for inclusion into USEtox, where they will undergo an independent evaluation process before any of them can be taken up in the consensus model.

USEtox developers have been addressing several suggestions for further adaptations and improvements of the model, as related to assessment of ecotoxicity, including:

1. better interpretation of the model outcomes;
2. clear communication of the applicability domain of the model, which includes 'expectation management' and 'avoidance of the probability of over-interpretation or expectation' of the current model results, given its focus on freshwater exposures;
3. consideration of additional substances and compartments, beyond freshwater;
4. improvements in the transparency in calculation of characterisation factors, from ecotoxicity data to final impact scores;
5. optimisation and added transparency regarding the selection of input data (physicochemical properties, degradation half-lives, ecotoxicological effect data) used to calculate the characterisation factors (CFs).

Ecotoxicity in LCIA has recently advanced through the third phase of the UNEP-SETAC Life Cycle Initiative flagship project launched to provide global guidance on environmental LCIA indicators (Jolliet et al. 2014). Within the flagship project, an Ecotoxicity Task Force (ETF) was formed to provide recommendations about the use or adaptation of existing models and/or factors for dealing with ecosystem exposure and effects of chemicals in LCIA where the science is sufficiently mature to ensure consensual recommendations. Building on previous recommendations, the following issues were identified by the ETF as priority tasks to consider for further improvements: i) the general assessment framework; ii) inclusion of additional compartments, exposed organisms, and impact pathways; iii) mechanisms influencing exposure to chemical substances; iv) speciation and long-term accessibility of metals; v) essentiality of metals; vi) ecotoxicity of chemical mixtures; vii) metrics for ecotoxicity characterisation; viii) disappearance of species from an ecosystem due to chemical exposure; and ix) meaning and interpretation of results. The issues associated with the general assessment framework, additional compartments (air and groundwater), and essentiality of metals were resolved during the initial stage of the flagship project, as presented in Fantke et al. (2018). Briefly, it was recommended to build on the current framework in LCIA, to consider ecotoxicological effects on freshwater sediment, soil, and coastal seawaters, and exclude consideration of ecotoxicological impacts on pollinators and essentiality of metals until the science is refined further to allow for that. Following the clearwater consensus recommendation about consideration of metal speciation in freshwater (Diamond et al. 2010), focus of the task force has naturally been on the consideration of metal speciation in other environmental compartments potentially relevant to include in the LCIA. The development of quantitative ion character–activity relationships (QICAR) for bioavailability factor (BF) calculations, although recommended by the clearwater consensus, has not been identified as a priority by the task force, as currently speciation models are available for many metals.

This chapter focuses on refining and expanding the consensus approach for ecotoxicity characterisation practice in LCIA given further matured scientific insights and data. First, we present the impact pathway for ecotoxicity and review related approaches and indicators. In line with the issues discussed in the ETF, the focus in the present chapter is on ecological exposure (including introducing additional compartments like sediment, coastal seawater, and soil) and ecotoxicological effects occurring in these compartments, while processes related to the environmental fate of chemicals are discussed in Chapter 4. Based on these discussions, we present the process for selecting approaches, provide consensual recommendations, and illustrate them in a practical case study. Processes influencing fate factor of a metal are outside the scope of this chapter as they are addressed in Chapter 4. Fate processes considered in USEtox 2.0 are also detailed in USEtox documentation (Fantke et al. 2017).

7.2 Impact pathways and review of approaches and indicators

7.2.1 Impact pathways

The impact pathway consists of:

1. fate modelling to determine the distribution of chemicals between environmental compartments, including degradation and transport processes like runoff, outflow to freshwater and oceans, leaching (referred to as environmental fate);
2. exposure of organisms to chemicals in the compartment of interest (i.e., ecological exposure);
3. potential ecotoxicological effects of chemicals on species assemblages in the various exposure compartments and resulting damage (i.e., ecotoxicity effects and damage).

Figure 7.1 illustrates the general impact pathway for ecological receptors from chemical emission to damage to ecosystems.

The first step in the impact pathway model is the release of the chemical substance into the environment. The ensuing environmental fate and exposure can be influenced by the substances' properties (e.g., solubility, persistence, and bioaccumulation potential) and co-determined by environmental characteristics (e.g., landscape parameters). For metals, environmental fate, exposure, and effects also depend on the metal forms of the primary emitted material (e.g., oxide, sulphide, elemental, etc.) (Ahnstrom and Parker 2001; Smolders et al. 2012), on ambient chemistry (like pH, concentration of organic carbon) that determines the ultimate solid- and liquid-phase speciation patterns of metals in environmental compartments (Degryse et al. 2009), and on the oxidation or reduction potential of the soil as determined by content of soil contents of oxides or organic matter and pH (Hooda 2010).

Upon their emission to a given environmental compartment (air, water, soil), a chemical usually ends up in one or more environmental compartments. Following fugacity principles, multi-media fate

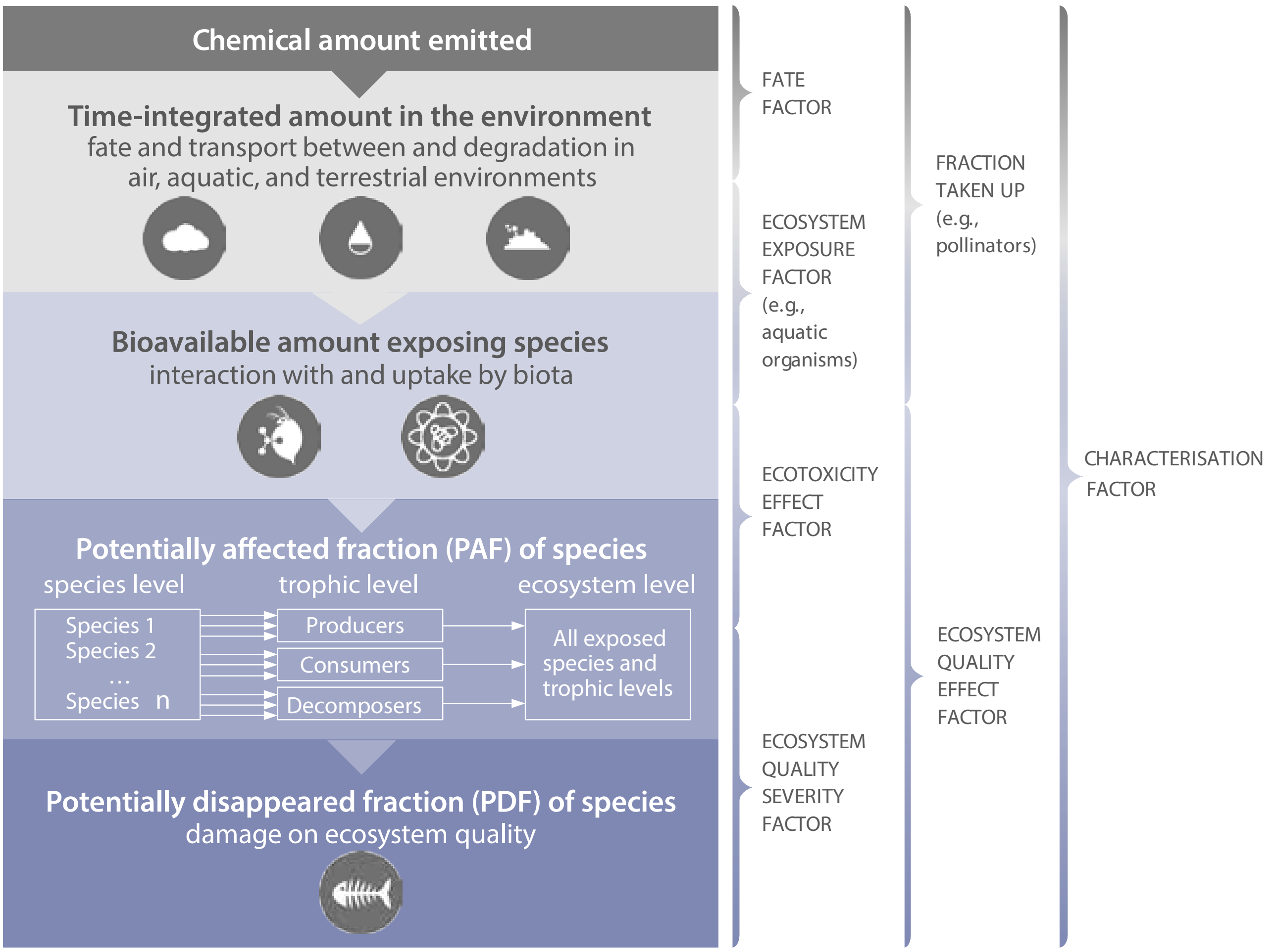

Figure 7.1. Impact pathway followed and framework for assessing ecosystem damage from emissions of chemical compounds (including metals and organics). Based on Fantke et al. (2018).

models are used in LCIA to predict steady state concentrations of chemicals in the various environmental compartments. Emission flow rate is used as the interface to LCIA multimedia models for calculating the fate factor, which expresses the predicted resident mass of a chemical in a receiving compartment per unit of emission flow into a given compartment. Higher values of the fate factor indicate higher persistence (Rosenbaum et al. 2008; 2011).

Once a substance is present in a given environmental compartment, exposure of organisms depends on the substance concentration that is actually available to cause exposure of the organisms' tissue due to uptake (depending on compound and environmental characteristics), as well as the exposure duration. In LCIA, the exposure factor (XF) represents the time- and space- integrated exposure of organisms to the bioavailable fraction of a substance in the compartment of interest.

To estimate the potential harm that a substance can cause, an ecotoxicity effects factor (EF) is used. The EF describes the ecotoxicological impacts on species in the environmental compartment due to exposure to the bioavailable fraction of a substance; higher values represent a higher intrinsic ability of the chemical to cause impacts for a selected fraction of the species representing the compartment of interest (capacity to cause harm), also referred to as the toxic pressure of an exposure, and expressed as potentially affected fraction of species (PAF, dimensionless). PAF is derived from species sensitivity distribution (SSD) curves (Huijbregts et al. 2002). To translate the toxic pressure metric to damage, a severity factor (SF) is applied to transpose the estimates of PAFs of exposed species to potentially disappeared fractions (PDF) of species. Furthermore, vulnerability factors can be used to weight individual species differently in different ecosystems.

Considering the impact pathway, a generic framework for calculating comparative ecotoxicity potentials is given (Jolliet et al. 2006; Rosenbaum et al. 2007):

$$CF_{i,s} = f_i \cdot FF_s \cdot XF_s \cdot EF_s \cdot SF_i \quad (1)$$

where $CF_{i,s}$ ($m^3/kg_{total\ emitted} \cdot d$) is the characterisation factor of a substance s emitted to compartment i; f_i ($kg_{total}/kg_{total\ emitted}$) is the fraction of substance *s* transferred in a steady state from emission compartment *i* to the compartment of interest; FF_s *(d)* is the fate factor calculated for total amount of substance *s* in the compartment of interest, equal to the residence time expressed in days of the substance *s* in that compartment[17]; XF_s ($kg_{available}/kg_{total}$) is the time-and space-integrated exposure factor that translates between the total mass of a substance in the compartment of interest and the available concentration that species are exposed to; and EF_s ($m^3_{water}/kg_{available}$, related to potentially affected fraction of species at given effect level) is the effect factor that represents ecotoxicological potency of the available fraction of substance *s*, and *SF* ($species_{lost}/species_{affected}$) is the severity factors that represents the severity of the effect in terms of damage on the ecosystem (that is, change in species biodiversity). The f_i is often integrated into emission-compartment specific $FF_{i,s}$.

Current ecotoxicity characterisation practice in LCIA (USEtox version 1.0) addresses impact pathways in freshwater and has not included a consensus approach for evaluating impact in freshwater sediment, soil, or marine compartments. While USEtox 1.0 focused only on the freshwater compartment, USEtox version 2.0 includes coastal water and soil compartments at the level of fate and exposure modelling. Meanwhile, the Uniform System for the Evaluation of Substances adapted for LCA purposes (USES-LCA) model, while not a consensus model, includes marine, soil, and sediment compartments at the level of fate, exposure, and effect modelling. Processes considered in USEtox 2.0 are detailed in USEtox documentation (Fantke et al. 2017).

7.2.2 Current approaches to addressing ecological exposure

While freshwater sediment, marine, and soil compartments are currently considered in multimedia fate models (Fantke et al. 2017; Van Zelm et al. 2009) current ecotoxicity characterisation practice in LCIA (USEtox 2.0) addresses only freshwater and does not yet provide a consensus approach for evaluating exposure in freshwater sediment, soil, or marine compartments. This section gives an overview of current practice in exposure modelling in various compartments, highlighting shortcomings and data gaps.

a. Freshwater

The exposure factors of chemical substances are usually calculated using approaches that consider major removal mechanisms, like sorption. Current practice in LCIA (e.g., in USEtox 2.0) is to express the

17 The f_i is sometimes coupled with the $FF_{i,s}$, depending on the fate model.

XFs as a truly dissolved fraction of total chemical, that is, as a fraction that is immediately available for uptake by an organism. The truly dissolved fraction (in USEtox 2.0 referred to as "fraction of chemical dissolved in freshwater") comprises all pools of a substance, which are not sequestered by association with suspended particles (SPs), dissolved organic carbon (DOC), or bioaccumulation in biota. Note, that the current practice assumes that the total substance reported in the inventory is available for these sequestration mechanisms, disregarding mechanisms like dissolution (of metals) or ageing or weathering.

For the vast majority of organic chemicals (except persistent highly adsorbing and bioaccumulating substances), affinity to SP, DOC, or biota is relatively small due to their relatively small octanol-water partition coefficients (Saouter et al. 2017). Moreover, since concentration of SP or DOC are often relatively small in freshwater compartment of current characterisation models, truly dissolved concentration in freshwater is in practice equal to total dissolved concentration (making XF equal to 1). This means that the total dissolved mass of many organic chemicals is in practice available for uptake by biota for the vast majority of organic substances. For lipophilic substances, however, XF in freshwater can be well below 1 (Saouter et al. 2017).

In the original version of USEtox (USEtox 1.0), the same practice of expressing the XF as truly dissolved fraction was applied to metals (including free ions and inorganic complexes, but excluding DOC- and SP-bound metal), and little consideration was originally given to the fact that metals exist as interconverting species of varying ecotoxicity, and that this speciation pattern is largely influenced by ambient chemistry. Furthermore, this definition of an XF in USEtox 1.0 was inconsistent with the definition of the EF that was based on total dissolved concentrations. Therefore, based on the work of Diamond et al. (2010) and Gandhi et al. (2010), the influence of ambient chemistry on speciation and resulting XF of metals, and matching XFs and EFs (that is, making their units compatible, expressed on a truly dissolved basis as computed using the Windermere Humic Aqueous Model (WHAM) combined with EFs derived using free ion activity models) are considered in USEtox 2.0 (Fantke et al. 2017).

Over the past few years, XFs were calculated for several other classes of chemicals, including pharmaceuticals, ionic and non-ionic detergents, ionic liquids, or nanoparticles. An overview of these studies is presented in Table S7.1.

b. Other compartments

USEtox 2.0 enables the calculation of XFs in coastal seawater and soil compartments. For coastal seawater, the formulation is the same as for freshwater, that is, sorption to SP, DOC, and bioaccumulation in marine organisms are considered as sequestration mechanisms. Concentrations of major cations influencing metal speciation patterns, like calcium, are not considered. For soil, where soil solids are the main sorbent, however, partitioning to soil gas and sorption to solid soil constituents are considered as sequestration mechanisms, but not sorption to DOC or SP in soil porewater. Although net sedimentation is considered in USEtox 2.0 as loss mechanism (that is, feedback from sediment to freshwater is considered in the fate factor), the model does not include freshwater sediment and related exposure as separate compartment. It is included, however, in the characterisation model USES LCA 2.0 (Van Zelm et al. 2009). The formula given in USES LCA 2.0 is similar to that of soil compartments, except the distribution to the gas phase is not relevant because sediment porewater is fully saturated with water. Recently, XFs have been calculated for metals in soil and coastal seawater compartments. An overview of these studies is given in Table S7.1. They follow approaches proposed earlier for freshwater, where liquid speciation is considered in the calculation of the XF (redefined as bioavailability factor), although it has to be noted that exact definitions of the bioavailability factor vary between studies (e.g., truly dissolved fraction of total metal, free ion fraction of reactive metal, etc.). In one study, solid-phase speciation of metals was considered (Owsianiak et al. 2015).

7.2.3 Current approaches to addressing ecotoxicological effects

In LCIA, EFs in aquatic systems are traditionally based on species sensitivity distribution (SSD) approaches, based on the observation that the sensitivities of different species for a chemical follow a normal distribution, which allow quantifying increased impacts with increasing exposures to yield a PAF-estimate for estimated exposures (Larsen and Hauschild 2007a; Larsen and Hauschild 2007b). The use of the SSD-model in LCIA was developed by Huijbregts et al. (2002) and others for comparative

LCIA. This principle has developed over time, so that the current approach is to estimate an EF based on an SSD-EC50 (an SSD derived from chronic lethal or effect concentration affecting 50% of the organisms [L{E}C50]). Linear concentration-response functions with 50% of the species affected as working point (percentile) on an SSD curve is most commonly used, so the resulting EF is defined as 0.5/HC50, where HC50 is the hazardous concentration of substance affecting 50% of the species. The non-linear concentration-response function is optional in USES LCA 2.0, but its consistent use in LCIA requires that the background pressure (in terms of PAF of species) from a chemical substance is known (Pennington et al. 2004). This information is currently not available for the vast majority of chemical substances and geographical locations.

In practice, $\log_{10}$(HC50) is calculated by first taking the geometric mean across available chronic L(E)C50 data points per species, and then taking the arithmetic mean of the logarithmic values for all species-specific chronic L(E)C50 geometric mean values (Fantke et al. 2017). The 50th percentile was found to be an appropriate basis for comparing chemicals in terms of contribution to cumulative risk in the presence of multiple stressors and background chemical mixtures (Pennington et al. 2004). This approach was already proposed by van Straalen and Denneman (1989) who described the 'forward' and 'inverse' use of SSD curves for deriving impact estimates from ambient exposures and protective criteria, respectively (an example of an SSD-based definition of environmental quality criteria is the predicted no effect concentration [PNEC] approach utilised in REACH). Although damage modelling in LCIA is based on the same data and modelling approach (SSD), it does not use conservative estimates and yields impact estimates. Indeed, it was later shown that the predicted PAF-EC50 (acute) correlates in a roughly 1:1 way, with the PDF on the basis of empirical associations between lab-based statistical predictions (PAF) and species loss attributed to chemical exposures (Posthuma and De Zwart 2006; Posthuma and de Zwart 2012).

The translation of PAF to the PDF (damage) level is made through an SF. Current practice in USEtox (based on the median of an SSD-chronic EC50) is to use a factor equal to 0.5, emphasising the importance of basing the SSD curve on chronic effect data. The factor of 0.5 means that a PAF-chronic EC50 of 10% of species affected over their level of chronic EC50 effect concentration is expected to lead to a species loss of 5% of the species due to toxic stress from chemical exposure (Jolliet et al. 2003). Recent approaches investigated empirical relations between predicted, laboratory-based, PAF-endpoint values and observed impacts attributed to chemicals via eco-epidemiological assessment methods. Both types of data are from different domains, though an increase in laboratory-based PAF-endpoint values (statistically derived metric based on lab data) is logically interpreted as a higher potential ecotoxicity stress, whilst the latter refers to field data. Various example studies suggest that the PAF-EC50 relates to damage (fractional species loss) (Posthuma and De Zwart 2006; Posthuma and de Zwart 2012).

Although current practice is to base SSD curves on chronic EC50 values (which in most cases are extrapolated from acute EC50 data), chronic ecotoxicity effect data are rarely reported as EC50s, and extrapolation of chronic EC50s from acute EC50s is not straightforward for all chemicals. SSD curves can also be constructed using no observed effects concentrations (NOECs), or impact endpoints such as EC10 or EC20 (as for EC50, representing increased effects of a chemical on vital traits such as growth and reproduction). Irrespective of the type of effect data underlying the SSD curve, however, it requires a new factor to "translate" a PAF, which in most cases is based on lab-data, to the damage expressed as PDF. Consequently, these approaches are operational at PAF level, but not yet at PDF level.

Although consensual recommendations on ecotoxicity effects in LCIA exist for freshwater only, some characterisation methods include effects of chemical substances on terrestrial and marine ecosystems largely based on extrapolating effect data from freshwater ecosystems (Goedkoop et al. 2009). For most organic chemicals there is no statistically significant difference in sensitivity (hazardous concentration, HC50) of aquatic and terrestrial organisms although in some cases there might be deviations of up to one order of magnitude (Golsteijn et al. 2013). The ratio of the soil porewater HC50/freshwater HC50 was typically 3.0 for narcotic chemicals (2.8 for nonpolar and 3.4 for polar narcotics), 0.8 for reactive chemicals, 2.9 for neurotoxic chemicals (4.3 for AChE agents and 0.1 for the cyclodiene type), and 2.5 for herbicides-fungicides (Golsteijn et al. 2013)

7.3 Process and criteria applied and process to select the indicator(s)

7.3.1 Process

A workshop was organised in May 2017 in Brussels as a starting point for developing recommendations about including additional compartments and impact pathways into existing characterisation approaches for ecotoxicity in LCIA. Findings from this workshop are summarised in Fantke et al. (2018). An ecotoxicity task force (ETF) was then formed with a remit to evaluate the maturity of science and the availability of effect data and extrapolation approaches. It consisted of 64 members who expressed a wish to be informed about the work carried out within the ETF, of which approximately 25% were members who actively contributed to the work.

Based on expertise and interest of the ETF members, two major subtask groups were identified and charged with investigating the following focus points:

1. exposure modelling across compartments, covering mechanisms influencing exposure of chemical substances, speciation, and ageing or weathering of metals; and
2. effects or damage modelling across compartments, investigating availability of freshwater sediment, soil, and marine effect data.

Issues associated with the meaning and interpretation of results were addressed by the whole ETF. Where applicable, the subtask forces identified criteria of good practice from the literature and carried out a review of new approaches for calculating CFs and underling XFs and EFs for various groups of substances and compartments of interest. Major features of new approaches are summarised in Tables S7.1-S7.4. Outcomes of the subtask groups were presented to the whole ETF during monthly conference calls between September 2017 and May 2018. Discussions within the ETF resulted in a preliminary set of recommendations, summarised in the ETF White Paper, which served as an internal document for communication as input to the Pellston Workshop in Valencia in June 2018. At the Pellston Workshop, seven experts discussed further recommendations presented in the ETF White Paper with regard to maturity of methods and availability of data, tested the feasibility of implementing some of the potentially recommended approaches on a case study, and proposed a final set of recommendations, which are presented in this chapter. For consistency with other impact categories addressed in the GLAM project, four recommendations levels (strongly recommended, recommended, interim recommended, and suggested/advisable), were used (Frischknech et al. 2017).

7.3.2 Generic criteria

Adopting the principle that model outcomes should relate to damage, expressed in PDF-related metrics, the approaches recommended were thus selected so they:

1. are feasible to implement, considering both the quality of data and the need for covering a large number of substances;
2. reflect the frontier of stable science, but not necessarily the spearhead science; and
3. are parsimonious, i.e., 'as simple as possible but as complex as needed,' adding value rather than uncertainty and unnecessary complexity (Hauschild et al. 2008a).

7.3.3 Specific criteria for ecological exposure factors

As a first step toward developing recommendations about ecological XFs, assessment of the maturity of existing approaches (that is, all new studies listed in Tables S7.1-S7.3), was done. Criteria were developed building on previous work from the UNEP-SETAC Life Cycle Initiative and from the development of recommendations for CFs under the ILCD project (Hauschild et al. 2013; European Commission 2011). This criteria address:

1. environmental relevance (like basing factors on effect data of certain types and qualities);
2. scientific robustness (e.g., inclusion of major exposure or effect mechanisms like speciation for metals) and certainty (like provision of uncertainty estimates);
3. documentation, transparency, and reproducibility (like being published in peer-review literature);
4. applicability (e.g., ability to link with life cycle inventory data).

Results of the evaluation of XFs calculated for various chemical substances in studies identified in a literature review against the aforementioned criteria are presented in Table S7.1. Three major observations are found: (i) no truly new approaches for calculating XFs for organic substances exist; (ii) XFs for novel entities (including ionic liquids, detergents, nanoparticles) largely build on USEtox as the underlying fate and exposure model; and (iii) the majority of approaches do not include all relevant mechanisms influencing exposure (with the exception of metals where speciation in the liquid phase was considered). Results of this evaluation were used as direct input to the Pellston Workshop where specific approaches were recommended.

7.3.4 Specific criteria for ecotoxicological effect factors

Five alternative approaches toward calculating EFs were assessed using assessment criteria building on previous work from the UNEP-SETAC Life Cycle Initiative and from the development of recommendations for CFs under the ILCD project (Hauschild et al. 2013; European Commission 2011). The following approaches were assessed: (i) HC50-EC50, (ii) HC5-NOEC, (iii) PNEC-NOEC, (iv) lowest validated endpoint (EC50, NOEC, or EC10) across at least 3 trophic levels, and (v) weighted average of lowest toxicity for 3 trophic levels. The criteria to characterise or judge the alternatives are:

1. general characteristics (like marginal or average damage);
2. completeness of scope;
3. compatibility (like fit to overall LCA framework);
4. applicability (e.g., implications for modelling exposure factors);
5. substance coverage;
6. fit of an SSD to data that is either statistically or biologically defendable;
7. the potential to link estimated PAF to PDF.

Results of the evaluation of these approaches to calculated effect factors against the criteria i-iv are presented in Table S7.4. Two major observation are that

1. PNEC-based approaches do not logically allow for damage modelling and hence, do not fit the LCA framework, and
2. the quantitative relation between estimated PAF and loss of species is not clear for the indicators based on lowest validated data value (EC50, NOEC, or EC10), obtained from tests with at least 3 trophic levels, and for the indicator based on weighted average of lowest toxicity for 3 trophic levels.

The overall conclusion was that other potential approaches in addition to the current HC50-chronic EC50, such as (potentially), HC20-EC50, HC50-EC10, HC20-EC10 can be considered as an effect indicator since any PAF-ECx is expectedly related to PDF due to its derivation principles. Hence, these alternative approaches were discussed at the Pellston Workshop focusing on the aforementioned criteria (see points 5-7). Updating here also involved a re-expression of these commonly used abbreviations, into the better option to express working points on SSDs as for example, P50-SSD-chronic EC50 (current approach) and P20-EC50, P50-EC10, etc., to define different usages of SSDs for LCIA, where P indicates the working point on an SSD curve.

7.4 Description of indicator(s) selected, models, methods, and specific issues addressed

7.4.1 Additional compartments

The ecotoxicity of chemical emissions should ideally be characterised in all relevant environmental compartments. Ranking of systems fulfilling the same function cannot be just based on freshwater impact scores because fate and exposure factors are likely to be different in those additional compartments compared with factors in freshwater. In this section, recommendations are made about inclusion of additional compartments in characterisation of ecotoxicity in LCIA.

a. Coastal seawater

It is recommended to include the ecotoxicological effects of chemicals on organisms living in coastal seawaters. If available, calculate an SSD-based effect factor using effect data for marine organisms. If absent or poor, combine with data from freshwater organisms, assuming equal sensitivity of marine and freshwater organisms (Leung et al. 2001; Wheeler et al. 2002). For metals and ionisable chemicals, effect data must be corrected for differences in speciation or dissociation patterns between coastal seawater and freshwater. In the communication of results, it should be noted that effect data for marine-specific phyla are virtually absent, so that they are not represented in the resulting EF. More insight into SSDs for marine species and relationships with SSDs for freshwater species is needed to make the recommendation strong.

b. Freshwater sediment

It is recommended to include the ecotoxicological effects of chemicals on organisms living in freshwater sediment. If available, calculate an SSD-based EF using effect data for freshwater sediment organisms. If absent or poor, combine with effect data from pelagic freshwater organisms, adjusted to reflect the bioavailable fraction of chemical in the porewater, assuming equal sensitivity of freshwater sediment and pelagic freshwater organisms (Di Toro et al. 2001). Again, more insight into SSDs for sediment species and relationships with porewater mediated SSD modelling for pelagic freshwater species is needed to make the recommendation strong. Pelagic freshwater organisms are preferred because extrapolations have been tested for pelagic organisms only.

c. Soil

It is recommended to include the ecotoxicological effects of chemicals on organisms living in soil. If available, calculate an SSD-based EF using effect data for soil-dwelling organisms. If absent or poor, combine with effect data from pelagic freshwater organisms, adjusted to reflect the bioavailable fraction of chemical in the soil porewater, assuming equal sensitivity of soil-dwelling and pelagic freshwater organisms. Again, more insight into SSDs for soil-dwelling species and relationships with porewater mediated SSD modelling for pelagic freshwater species is needed to make the recommendation strong. Pelagic freshwater organisms are preferred because extrapolations have been tested for pelagic organisms only.

We acknowledge that the recommended extrapolation approaches might not work equally well for some individual substances with specific modes of action towards some organisms living in, and specific to, the compartment of interest. In this case, particular attention is needed when applying the recommended standard procedures in the future. Currently, it is not known for which specific substances deviations from standard procedures may apply. To ensure that the aforementioned recommended approaches are used wisely, **it is strongly recommended to consider specific characteristics of chemicals, organisms, and compartments during the calculation of effect factors if information about them is available**. This could imply deviations from the recommended standard LCIA procedures, so that the resulting EF reflects the state of the science. This recommendation is a consequence of the huge variety of chemicals, compartments and organisms to be considered. Any such deviation shall be transparently documented and justified in the reporting.

7.4.2 Ecological exposure factor

Recommendations are made regarding the consideration of bioaccumulation in modelling exposure of chemical substances across all compartments, and regarding the mechanisms influencing exposure of metals (namely, liquid and solid phase speciation).

a. Bioaccumulation of chemical substances

Bioaccumulation is currently considered a sequestration mechanism when calculating XFs in freshwater and coastal seawater but not in soil (USEtox version 2.0) or freshwater sediment (USES-LCA 2.0). Current formulation of the XF considering bioaccumulation as sequestration mechanism is consistent with ecotoxicological EFs if they are derived using chronic field data, as was prioritised in USEtox. However, chronic field data is rarely available, and for the vast majority of substances, EFs are derived from laboratory experiments measuring acute endpoints. For some highly bioaccumulating substances like the fungicide fludioxonil, the fraction of the chemical present in biota at steady state that is predicted using USEtox 1.01 can be higher than 10% (Saouter et al. 2017). Thus, for highly bioaccumulative substances, CFs are underestimated when bioaccumulation is not considered in the related effect data. To harmonise exposure modelling across compartments and to make XFs and EFs more consistent, **it is strongly recommended to disregard removal through uptake into biota when calculating the exposure factor.** Bioaccumulation must be included, however, when calculating fate factors and if chemical transfer to higher trophic levels is considered.

b. Liquid-phase speciation and solid-phase accessibility of metals

Metal exposure is largely determined by ambient chemistry as it influences liquid phase speciation patterns of the metal in the water phase of the compartment of interest (Van Leeuwen 1999). In addition to the liquid phase speciation, the solid-phase accessibility (here, exchangeability based on geochemistry, describing the potential for solid-liquid partitioning within a time scale of days) (Degryse et al. 2009), as influenced by ageing and weathering reactions, is particularly relevant for metals in soil or sediment. It determines which fraction of the metal pool in the soil is potentially accessible for leaching and uptake by biota (Ehlers and Luthy 2003). To make the assessment of metals more environmentally relevant, **it is strongly recommended to consider liquid phase speciation as mechanisms influencing exposure and effects for metals in coastal seawater, freshwater sediment, and soil.** As a consequence, the spatial variability in ambient chemistry parameters, including spatial variability in background concentrations, as CFs vary nonlinearly with background concentrations, has to be considered when calculating XFs for metals (Diamond et al. 2010). **Furthermore, it is strongly recommended to consider metal accessibility in soil as influenced by ageing and weathering mechanisms for uptake into biota, when characterising exposure of soil-dwelling organisms. It is also interim recommended to consider metal accessibility in freshwater sediment as influenced by ageing and weathering mechanisms for uptake into biota, when characterising exposure of sediment organisms.** This recommendation is interim due to limited insight into ageing and weathering patterns of metals in freshwater sediment.

For coastal seawater, these recommendations are consistent with XFs calculated by Dong et al. (2016) for a set of 64 large marine ecosystems, which were expressed as bioavailability factors (here, proportion available for uptake expressed as truly dissolved fraction of total metal in coastal seawater). For soil, these recommendations are consistent with the method of Owsianiak et al. (2013a, 2015) who defined the XF as a product of the bioavailability factor and the accessibility factor. A meta-analysis study for selected cationic metal emissions of anthropogenic origin showed that at timescales of decades to centuries, the influence of time on accessibility of anthropogenic metals in soils is difficult to capture based on empirical studies and is statistically uncertain (Owsianiak et al. 2015). Models that allow predicting time-dependent changes in the reactive fraction in soil are available, but they do not consider long-term (>3 years) ageing mechanisms as they were developed for readily soluble metal salts, and overestimate the reactive fraction of metals in the soil (e.g., Buekers et al. 2008; Crout et al. 2006). Hence, in the absence of ageing or weathering models for anthropogenic metal forms, an accessibility factor derived from reactive fractions measured at various points in time, as done by Owsianiak et al. (2015), can be used. The Soil PNEC Calculator of Arche contains potentially useful data, but the approach presented in the calculator is not deemed optimal for LCIA. The calculator corrects for ageing (and leaching) basing on experiments with spiked soils aged for relatively short-term (up to 18 months). In the LCIA context, an approach that can be applied to metal emitted in anthropogenic (mainly solid-phase) forms and captures long-term (centuries) ageing and weathering mechanisms, is more relevant. While some advances in research into ageing and weathering patterns of metals in freshwater sediment have been reported (Costello et al. 2015; Costello et al. 2016), insights are yet too scarce to support any recommendation about time-dependent changes in solid phase speciation in this compartment.

No specific recommendations are made about whether free ion concentration or truly dissolved concentration (including free ions and inorganic complexes) shall be used as descriptor of exposure in the calculation of bioavailability factors, provided that units of exposure factors are consistent with unit of effect factors (that is, expressed basing on the same bioavailable metal pool).

No specific recommendations are given on how to specifically consider spatial variability in the exposure and resulting CFs. This will vary, depending on the compartment of interest. If a site-specific inventory of emissions is available for application in regionalised LCA, spatial variability in the exposure factor (and resulting characterisation factor) could be considered by either computing site-specific factors for the site of well-defined chemistry parameters, as done for soil by Owsianiak et al. (2013), or assigning a site-specific characterisation factor to a given archetype (e.g., soil of properties representing typical chemistry), or ecosystem type as done for soil (Plouffe et al. 2016) or coastal seawaters (Dong et al. 2016). For use in generic LCA, archetype-specific CFs could be weighted based on occurrence of each archetype in the world (e.g., Dong et al. 2014). Alternatively, a generic CF could be chosen from a set of spatially explicit CFs, based on the proximity of the properties of environment, for which a spatially explicit factor was calculated to properties of the generic compartment in a multimedia fate model.

7.4.3 Ecotoxicological effect factors

Recommendations are made about the choice of ecotoxicity data and on modelling toxic pressure (PAF) and damage (PDF).

a. Link to ecosystem quality damage

LCIA must enable evaluation of expected damage to species assemblages that results from the emission of chemical substances from a product system and must enable a comparison of damages with damages due to other stressors (that is, stressors not contributing to ecotoxicity but with potential to cause harm via other mechanisms). **It is therefore strongly recommended to base damage on potentially disappeared fraction (PDF) of species.** Recent studies show that there is a nearly 1:1-type relationship between the (mixture) toxic pressure (msPAF-EC50) and the species PDF for various species groups, suggesting that similar relationships are expected to hold between the mixture toxic pressure derived from other types of effect data, including chronic effect data (Posthuma and De Zwart 2006; Posthuma and de Zwart 2012).

b. Ecotoxicity indicator

Relative sustainability, as assessed using LCA, is concerned with long-term implications of emissions on receiving ecosystems. It is therefore natural to use chronic effect data as a more accurate (albeit potentially less certain due to fewer available test data to derive SSDs, except some metals) indicator of long-term damage to ecosystem. LCA is not concerned with acute, short-term impacts because of their very site-specific and dynamic nature; high concentrations of chemicals are seen very locally around emission outlets and for short periods of time. It is argued, however, that the current practice does not necessarily ensure a fair comparison between chemical substances – and other stressors – because the current working point P50-SSD-EC50 is commonly far from the domain of environmental (ambient) concentrations (unlike the common practice for other stressors in LCIA) (Posthuma and De Zwart 2006; Posthuma and de Zwart 2012). Moreover, the shape of the SSD curve varies between different chemical compounds, depending on their mode of action towards specific organisms included in the SSD curve and on ambient concentrations (Posthuma et al. 2001; Belanger et al. 2017; Posthuma et al. 2018). Hence, concerns are raised that in a comparative LCIA context, there is a risk that impact-determining information may be lost about particularly toxic (or particularly nontoxic) chemical substances at environmentally relevant concentrations if 50th percentile is used as the working point on the SSD curve. **It is therefore recommended to base effect modelling on a concentration domain of the SSD curve that is close to the domain of environmental (ambient) concentrations. It is recommended to use the 20th percentile as the working point on the SSD curve. It is recommended to derive the SSD curve using chronic EC10-equivalents as underlying effect data to estimate the potentially affected fraction of species (PAF).** To make the recommendation strong, the SF linking PAF-EC10-equivalents and species PDF in the environment must be established. The chronic EC10-equivalent is considered equivalent to the chronic endpoints NOEC, LOEC, MATC, EC50, and chronic ECx where x is between 1 and 20, converted from e.g., ECx to EC10 using a correction depending on the exposure level x. Specification of these is pending based on existing sources of literature. Acute to chronic extrapolations are to be used to fill in data gaps to increase coverage of species and substances. Given current variations in ambient concentrations, both the EC10-endpoint as well as the 20th percentile of the SSD used for impact modelling are closer to ambient concentration than the currently applied metrics (the 50th percentile of the SSD-EC50) (e.g., de Zwart et al. 2011). The 20th percentile was selected because five data points (five species) are sufficient to derive an HC20 value without the need to extrapolate the SSD beyond the existing data. Calculating a non-extrapolated HC10 would require data for ten different species, an amount of data that is most likely not available for the majority of chemicals. If the number of species is below five, a read across procedure can be explored, where an SSD is constructed from the 50th percentile (HC50) calculated as geometric mean of species EC10-equivalents and assuming a generic shape of SSD based on current knowledge of SSD curves for substances with the same model of action to derive HC20 values. Currently, no recommendations are made about which shape to assume at this point as more research is needed. Chronic EC10-equivalents are further chosen instead of chronic EC50 values because the number of reported ecotoxicological effect data, which are close to EC10 (like NOEC, LOEC) is larger compared with chronic EC50 values. Furthermore, chronic EC50 values are not expected to be generated to a large extent in the future. EC10-equivalent is aligned with the use of ED10 as a reference point on the dose-response curve recommended by the human toxicity task force (Chapter 4).

Considering the dynamic nature of some of the ecotoxicity databases underlying SSDs (where data can be added or removed at any time, such as in the REACH database), it is important to ensure the reproducibility of EFs. This means that raw data underlying the calculation of EFs, retrieved from a database at any given point in time, can be retrieved again at any future point in time, irrespective of how the database has evolved. **It is strongly recommended that the data used to calculate effect factors have a traceable origin.** This is to introduce transparency and allow for updates as science and data availability develops.

c. Ecotoxicity effect modelling of metals

Metals can exist as a dynamic species of varying ecotoxicity as determined by ambient chemistry like the concentration of dissolved organic carbon or pH (Van Leeuwen 1999). When expressed based on bioavailable concentrations (e.g., free ion or truly dissolved), metal ecotoxicity depends on concentration of protons (pH) and dissolved ions (e.g., calcium, magnesium) in the water phase of the compartment of interest (Di Toro et al. 2001; Thakali et al. 2006a)

Current LCIA practice for freshwater (i.e., USEtox version 1.01) is to calculate EFs for metals using free ion activity models (FIAM), which are derived from ecotoxicological effect data by means of speciation modelling (Campbell 1995). At the time when USEtox was developed (version 1.0), FIAMs were utilised due to the unavailability of biotic ligand models (BLMs) for all metals. Even though BLMs were recognised to be more accurate, the use of FIAMs was preferred to ensure consistent treatment of all metals. It was shown that estimates of CFs from FIAMs were comparable to those from BLMs for metals for which BLMs were available then (Gandhi et al. 2011) in freshwater ecosystems. Dong et al. (2014) showed that for some metals, the differences between FIAM-based and BLM-based CFs can be large (up to 1 order of magnitude), depending on the freshwater type and its chemistry. While BLMs have been shown to be a better predictor of ecotoxicity (Santore et al. 2017), and more BLMs have been developed in recent years for some metals, FIAM ensures consistent treatment of all metals for many organisms in all compartments.

Current LCIA practice disregards the influence of ambient chemistry in the calculation of metal ecotoxicological EFs in other compartments than freshwater. To improve current practice, **it is strongly recommended to use free ion activity models in the calculation of effect factors for metals in soil, freshwater sediment, and coastal seawater compartments.** Free ion activity models are recommended because they can be derived via speciation modelling for the majority of metals for which free ion is the major toxic metal form, and they allow for the consistent ranking of metals in terms of their ecotoxicity. More advanced aquatic and terrestrial BLMs are available for a few metals (Ardestani and van Gestel 2013 and references therein), but it was decided not to consider them, as their use could lead to a bias in metal ranking and ratio of CFs between metals when combined with those metal for which BLMs are not available. The recommended practice is consistent with that of Dong et al. (2016) in coastal seawater, and is partly consistent with Owsianiak et al. (2017) for soils, who used FIAMs for those metals for which terrestrial BLMs were not available in large quantities.

7.4.4 Interpretation and communication

Though the focus of the ETF was on exposure, effect, and severity components of the ecotoxicity CF, it is important to consider implications of the way the fate factor is calculated on the interpretation of CFs and resulting impact scores. Following the discussion on fate factor, recommendations are made about the presentation of ecotoxicity impact scores, their interpretation and units.

a. Interpretation of ecotoxicity characterisation factors and related impact scores

It is incorrect to assume that using an infinite time horizon when calculating fate factors and resulting CFs implies a bias that neglect potential impacts of fast-degrading organic substances, or that such use neglects to consider short-term impacts. Despite the assertion of Saouter et al. (2018), chemicals that adsorb on suspended particles and that move to sediment, to dissolved organic carbon, bioaccumulate, or substances of high volatility are included in the final impact score. In freshwater, the fate factor represents the change in steady-state substance amount in the water column that results from a unit change in the emission mass flow rate into freshwater or any other compartment (with a unit of $kg_{in\ freshwater}$ per $kg_{emitted}$/day). The emission flow rate is used as an interface to LCIA multimedia models for calculating the fate factor. Because multimedia fate models applied in LCIA use constant coefficients, the steady-state concentration is a linear function of the emission flow rate. Hence, a change in steady-state substance amount in the water column that results from a unit change in the emission flow rate is mathematically equivalent to the overall cumulative amount from a pulse emission, accounting for the environmental residence time of the substance (Heijungs 1995). Graphical interpretation of the fate factors including example calculations is presented in Figure **S7.1**. Therefore, both short-term and long-term impacts are considered (with equal weight), even if infinite time horizons are used to calculate fate factors and resulting characterisation factors.

As for interpretation, ecotoxicity impacts assessed in LCIA are not directly observable for two reasons, as argued in Hauschild and Huijbregts (2015):

1. elementary flows which have been attributed to the functional unit (e.g., consumption of 1 kg of rice) are generally aggregated over time and space, while observable impacts on ecosystems are usually measured at specific points in time and space; and
2. we do not know simultaneous emissions from other processes which expose the same ecosystems and emissions of other stressors causing harm to ecosystems.

Recent research has shown that chemical exposures are a limiting factor to the possibility to maintain reference-state biodiversity, that is, ecotoxicological effects may be masked by other factors, for example, eutrophication may mask the impacts of toxic chemicals (Barmentlo et al. 2018). Therefore, although being a damage indicator, the PDF is to be interpreted as a capacity to cause harm, rather than a numerical estimate of materialization of harm. Impact category indicator results should be interpreted as relative performance indicators, which can be used to optimise given product systems and compare with other systems fulfilling the same function (while considering uncertainty and variability sources) (Douziech et al. 2019), rather than indicators of real effects on the environment. As argued further in Hauschild and Huijbregts (2015), product systems assessed in LCA cannot be monitored in the real world. Thus, CFs cannot be validated, though they can be empirically evaluated by comparing predicted toxic pressures and observed mixture impacts. Validity of use of CFs can be further ensured by using data and models (underlying calculations of CFs), which have been validated. **It is strongly recommended to stress, when interpreting impact scores, that scores represent the time- and space- integrated potential, but not the actual, ecotoxic impact on receiving ecosystems**

b. Presentation of ecotoxicity impact scores

A challenge for LCA practitioners who need to interpret results to support decisions is identifying all relevant substances contributing to the ecotoxicity impact score. To support this interpretation, **it is strongly recommended to present impact scores on a $\log_{10}$-scale.** This relates to the fact that CFs can vary between different chemical substances by approximately 8 orders of magnitude in freshwater, and their uncertainty can vary by approximately 2-3 orders of magnitude in USEtox (Rosenbaum et al. 2008) or significantly higher (up to 7 orders) if all sources of uncertainty are considered (Douziech et al. 2019).

Metals often dominate total impact scores (for example, median contribution of cationic metals to total terrestrial ecotoxicity impact scores was 80% for ReCiPe 2008) (Owsianiak et al. 2017), while organic substances may be also relevant for decision-makers, depending on the goal and scope of the LCA. **It is furthermore strongly recommended to present impact scores separately for organic and inorganic compounds (including metals), while keeping them on the same ($\log_{10}$-transformed) scale.** Moreover, to avoid any potential misunderstandings of the interpretation of CFs and resulting impact scores, **it is an interim recommendation to present time integrated impact scores differentiated for time horizon periods, e.g., for the first 100 years, and beyond 100 years, which can be summed up to a total score.** To operationalise this recommendation, the appropriate number of time steps and their duration (e.g., 100 years) need to be defined. This recommendation is particularly relevant for metals, due to their longer residence times when compared with the vast majority of organic chemicals.

Current practice is to present unit of CFs, which includes PAF integrated over space (volume of the water in the compartment of interest) and time, per unit emission, so PAF•m^3•kg^{-1}•day (with higher values just implying high potential to cause harm). Since this unit is not so straightforward to interpret by LCA practitioners and decision makers, **it is recommended to communicate the unit of impact score as the comparative toxic units for ecotoxicity (CTUe); where** 1 CTUe is equal to 1 PAF•m^3•kg^{-1}•day. A system with a higher CTUe has a higher potential to cause species loss. A higher CTUe can be due to higher persistence, higher exposure, higher toxicity, or a combination of these.

Table 7.1. Characterisation factors (in CTUe/$kg_{total\ emitted}$) and underlying fate factors (in $kg_{total\ in\ compartment}/kg_{total\ emitted}\cdot day$), exposure factors (in $kg_{bioavailable}/kg_{total\ in\ compartment}$), and effect factors (in $m^3_{water}/kg_{bioavailable}$; where water refers to porewater for soil and sediment compartments) in three compartments. They were calculated for infinite time horizon using recommended approaches (that is, disregarding bioaccumulation as removal mechanism and using 20th percentile of SSD-EC10eq) for unit emission to each of the compartments. In the absence of effect data for marine and soil ecosystems, they were extrapolated from freshwater effect data as recommended. Colour coding was used to illustrate differences in factor values across compartments (increasing shade of orange reflects increasing factor value ; increasing shade of violet reflects decreasing factor value).

Cas	Substance	Characterisation factor			Fate factor			Exposure factor			Effect factor		
		Freshwater	Coastal seawater	Natural soil	Freshwater	Coastal seawater	Natural soil	Freshwater	Coastal seawater	Natural soil	Freshwater	Coastal seawater	Natural soil
141-43-5	Monoethanolamine	2810	3280	65.4	18.5	20.4	42.4	0.999	1	0.01	152	152	152
71-43-2	Benzene	1100	11100	328	4.28	37.8	10.7	1	1	0.119	258	258	258
67-56-1	Methanol	4.07	5.46	3.18	9.28	12	9.73	1	1	0.736	0.438	0.438	0.438
108-38-3	m-Xylene	1320	6370	132	4.06	18.6	9.91	0.999	1	0.041	324	324	324
100-52-7	Benzaldehyde	6560	16000	4010	8.62	19.8	18.9	1	1	0.279	760	760	760
137-26-8	Thiram	850000	1210000	5380	37.9	47	21.3	0.999	1	0.011	22400	22400	22400
100-41-4	Ethylbenzene	1620	7840	161	4.06	18.6	9.4	0.999	1	0.043	399	399	399
64-17-5	Ethanol	28.2	37.7	23.2	9.31	12	9.16	1	1	0.829	3.03	3.03	3.03
95-50-1	1,2-Dichlorobenzene	7970	73200	1240	5.01	39.1	37.6	0.998	1	0.021	1590	1590	1590
107-31-3	Methyl formate	33.7	165	45.8	4.3	18.8	6.91	1	1	0.849	7.78	7.78	7.78

7.5 Characterisation factors (except, including qualitative and quantitative discussion of variability and uncertainty)

Exposure, effect, and characterisation factors in freshwater, coastal seawater, and soil compartments were calculated for a selected set of organic substances from the large set of substances associated with the rice case study (Table 7.1). The choice of these substances from the larger pool was dictated by the availability of effect data in the freshwater compartment at the time when calculations were made, which were extracted from the REACH database. Fate factors were calculated for infinite time horizon using USEtox, v 2.0. EFs were calculated disregarding bioaccumulation as sequestration mechanism (recommended approach). Freshwater ecotoxicity EFs were calculated using the P20-EC10eq as indicator (recommended approach). Extrapolation factors to arrive at EC10eq published by Warne et al. (2015) were used. For two out of 12 substances data for less than five species were available. Therefore, freshwater effect factors were not calculated for these substances since read-across procedure were not yet operational. Insufficient effect data for marine and soil organisms were available at the time when calculations were carried out to derive effect indicators based on P20-HC10eq. Thus, following the recommended practice, extrapolations were done from freshwater effect data assuming that sensitivities of organisms in respective compartments are the same as those in the freshwater compartment.

Exposure factors are close to 1 kg/kg in freshwater and coastal seawater for all substances and range from 0.01 (ethanolamine) to 0.85 kg/kg (methyl formate) in soil. Effect factors vary 5 orders of magnitude and are smallest for methanol (0.438 m^3/kg) and largest for thiram (a pesticide) (22400 m^3/kg). Characterisation factors vary by 5 (freshwater and coastal seawater) and 3 (soil) orders of magnitude (for emission to these compartments). The substances with the largest and the lowest potential to cause harm in all compartments are thiram and methanol, respectively (per unit emission to the same compartment). The CFs generally increase in coastal seawater and decrease in natural soil when compared to CF values in the freshwater compartment. This is due to their different exposure factors (soil) and/or fate (soil and coastal seawater) in these compartments when compared with freshwater. For example, CFs are up to 8 times larger in coastal seawater when compared with freshwater due to higher fate factors. Fate factors can also be higher in soil when compared with freshwater, but exposure factors are usually smaller because of sorption to solid soil constituents. Uncertainties were not quantified in this illustrative exercise, but it is known that they vary 2-3 orders of magnitude in freshwater. This means that differences in characterisation factors of 6 orders of magnitude, as observed here between methanol and thiram in freshwater, are most likely significant. By contrast, difference by several orders of magnitude, as observed between several substances should not be interpreted as evidence for a significant impact difference.

7.6 Rice case study application

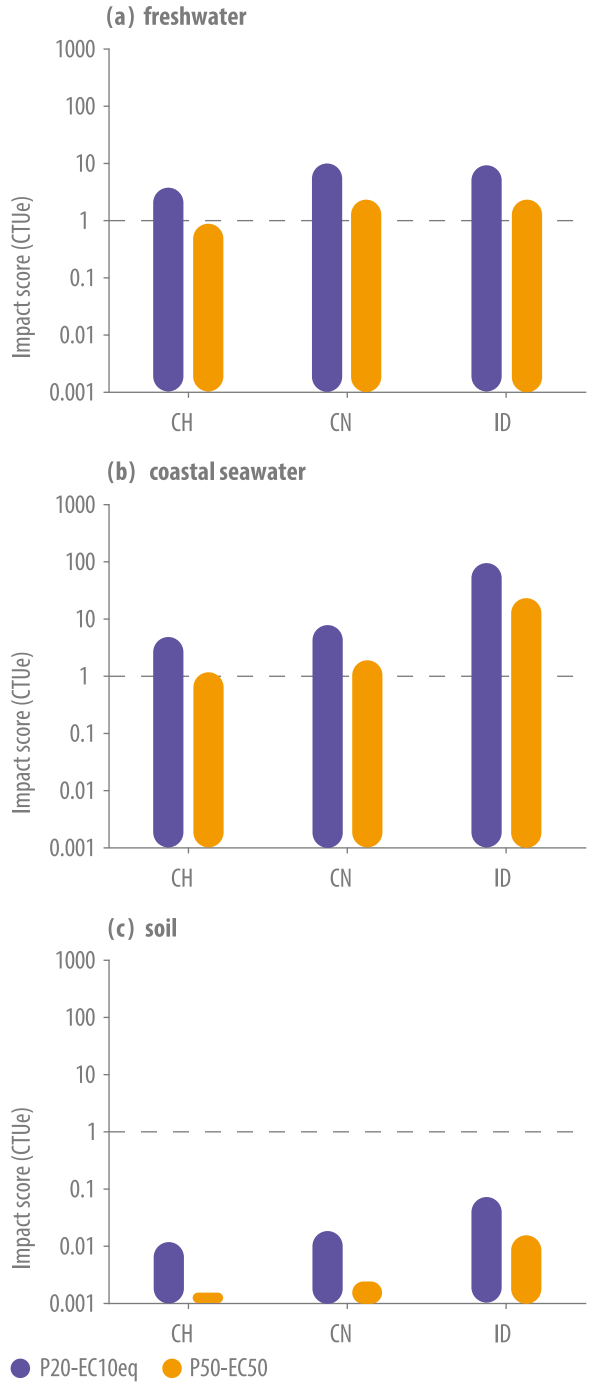

Figure 7.2. Freshwater (a), coastal seawater (b), and terrestrial (c) ecotoxicity impact scores calculated for selected substances reported in emission inventories in the rice case study using recommended (P20-EC10eq) and current (P50-EC50) practice. CH-Switzerland/US scenario; CN-China scenario; ID-India scenario. P indicates working point on an SSD curve.

Figure 7.2 shows ecotoxicity impact scores per functional unit defined as "1 kg of cooked white rice consumed at home" calculated for the three scenarios of the case study (China, Switzerland/USA, and India [Frischknecht et al. 2016]). Figure 7.3 shows substance contribution to each impact category for the China scenario. Only those substances for which characterisation factors could be calculated (see Section 7.5) were considered. Following the recommendations, impact scores are presented in $\log_{10}$-transformed scale. As no P20-EC10eq-based effect factors are yet available for metals, no metal was considered in the case study. Further, because fate factors in freshwater, coastal seawater, and soil of the organic substances included in this study are very small (below 50 days), the interim recommendation to present time integrated impact scores separately for different time horizon periods was not implemented.

For each scenario, comparisons were made with impact scores derived from characterisation factors calculated using current practice (that is, P50-EC50 and with bioaccumulation considered as removal mechanism). The following observations relevant for optimisation of product footprint reduction related to potential ecotoxic impacts are made:

a) The inclusion of new compartments adds information and decision support value, even if extrapolation from freshwater had to be made. For example, monoethanoloamine was identified as a potentially problematic substance in the soil compartment, despite using freshwater effect data as the basis for calculating the terrestrial effect factor. Similarly, benzene emitted to air was found to be the largest contributor to seawater ecotoxicity impacts. Differences in potential impacts caused by these substances were up to 5 orders of magnitude higher when compared with least-contributing substances.

b) Using the recommended approach, the numerical estimates of the impact scores (without SF) are higher by approximately 0.5-1 order of magnitude at midpoint compared with current practice. Note, however, that at endpoint, impact scores are expected to be comparable to those calculated using current practice because the net outcome of the PAF-Px/ECx to PDF from the newly recommended approach must be implemented with a newly derived PAF-PDF relationship (amending the current PDF=0.5xPAF). The link to PDF must be established to calculate characterisation factors at endpoint.

c) In this comparative, limited case study, there were no differences between conclusions drawn using current practices or recommended approaches. Impact scores appear largest for the India scenario, although differences in impact scores between scenarios are close to or below 2 orders of magnitude, suggesting that they might not be statistically significant from each other.

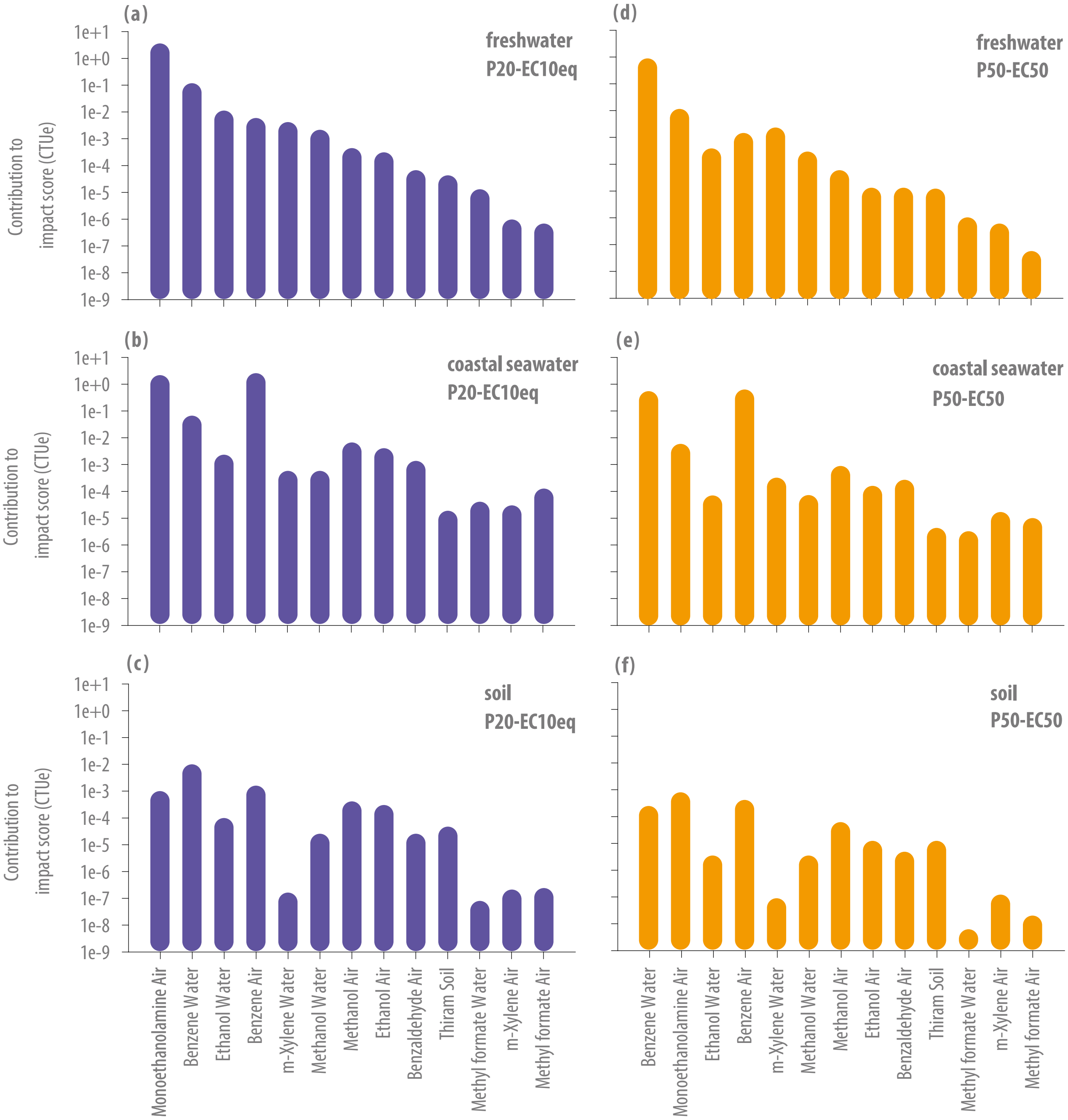

Figure 7.3. Contribution of the selected organic substances reported in emission inventories in the rice case study (China scenario) to freshwater, coastal seawater, and terrestrial ecotoxicity impact scores calculated using recommended (P20-EC10eq) (a-c) and current (P50-EC50) (d-f) practice. X-axis legends include substance name and emission compartment. P indicates working point on an SSD curve.

Table 7.2. Issues addressed by the ecotoxicity task force and summary of related recommendation. Three levels of recommendations apply: SR (strongly recommended); R (recommended); IR (interim recommended). The fourth level S/A (suggested/advisable) was used when developing recommendations, however upon concluding no recommendations were categorised at this level.

Issue addressed by the ecotoxicity task force	Brief summary of the recommendation	Level of the recommendation
General assessment framework	"Build upon the current framework in LCIA for assessing ecosystem damages from emissions of toxic chemicals" (Fantke et al. 2018)	SR, as agreed on before the Pellston Workshop
Inclusion of compartments, exposed organisms, and impact pathways	Include ecotoxicological effects of chemical substances on organisms living in freshwater sediment, soil, and coastal seawaters in LCIA	R
	Consider specific characteristics of chemicals, organisms, and compartments during the calculation of effect factors	SR
	Develop methods to address pollinator exposure and related impacts in LCIA due to the importance of this impact pathway (Fantke et al. 2018)	SR, as agreed on before the Pellston Workshop
Mechanisms influencing exposure to chemical substances	Disregard bioaccumulation as removal mechanisms in all compartments when calculating exposure factors	SR
Speciation and long-term accessibility of metals	Consider liquid phase speciation on metals in the calculation of exposure factor in freshwater, coastal seawater, soil, and freshwater sediment	SR
	Consider solid phase speciation (accessibility) in the calculation of exposure factor for metals in soil	SR
	Consider solid phase speciation (accessibility) in the calculation of exposure factor for metals in freshwater sediment	IR
Essentiality of metals	"Essentiality is recognized but of low relevance for LCIA ecotoxicity characterization, since ecotoxicological effects on some (sensitive) species can always be characterized independently of 'fertilizing' effects on other species at the same concentration range" (Fantke et al. 2018)	SR, as agreed on before the Pellston Workshop
Chemical mixture toxicity	Sum up impact scores across chemicals "as a first approximation for handling mixture toxicity under the typical situation of unknown chemical emission location and time along product life cycles" (Fantke et al. 2018)	SR, as agreed on before the Pellston Workshop
Metrics for ecotoxicity characterisation	Calculate effect factor from HC20 derived using SSD model constructed using chronic EC10-equivalents	R
	Use free ion activity models to calculate effect factors for metals	SR
	Use data that has a traceable origin	SR
Disappearance of species from an ecosystem due to chemical exposure	Base damage on potentially disappeared fraction of species. However, the link between fraction affected and fraction lost must be established.	SR
Meaning and interpretation of results	When possible, present impact scores on a log10-scale	SR
	Present impact scores separately for organic and inorganic substances	SR
	Present impact scores separately for different time horizons	IR
	Stress when interpreting results that impact scores represent time- and space-integrated potential (not actual) ecotoxic impact on receiving ecosystems	SR
	Use comparative toxic units for ecotoxicity (CTUe) as unit of impact score	R

7.7 Recommendations and outlook

a. Main recommendation – Short summarising theses

A brief synthesis of all recommendations (including strong and interim recommendations), which were presented in detail in section 7.4, is given in Table 7.2.

b. Judgement on quality, interim versus recommended status of the factors and recommendation

The recommendations are final. The characterisation factors presented in the report are for illustrative purposes only and shall be considered interim until procedures for data compilation and data curation are agreed upon. An additional effort is currently undertaken to collate, curate, and utilise at least three data sets: the US-EPA Ecotox database, which is an open source database with transparent data origins; the JRC-ECHA/EFSA database, which is not open source and has non-traceable data originating from the ECHA registration dossiers; and the SOLUTIONS-database, which also contains the non-traceable data from the ECHA registration dossiers (Posthuma et al. 2018). Some modelling tools, like the Soil PNEC calculator for metals offered by Arche (www.arche-consulting.be) should also be considered when collecting ecotoxicity effect data.

c. Applicability and maturity and good practice for factors application

Caution is needed when applying resulting characterisation factors for metals in freshwater and coastal seawater compartments, as the link between inventory and impact assessment is not obvious. Although the recommended factors consider liquid phase speciation in all compartments, various chemical forms of a metal can present in the emission flow dependent on the type of emission source. This is currently not considered in freshwater and coastal seawater compartments. In other words, it is assumed that metal will behave in freshwater or coastal seawater exactly the same way as it does in the speciation models underlying the calculation of the characterisation factors (where total metal is assumed to be available for solid-liquid distribution and liquid phase speciation). In reality, this will depend on the metal species that are emitted, which in current inventory practice is not known, and the kinetics of transformation reactions that they undergo in the environment.

For soil, this issue is resolved by introducing an accessibility factor into the characterisation factor, which provides a link between inventory and impact assessment phases (Owsianiak et al. 2015; Sydow et al. 2018). An accessibility factor is also relevant for freshwater sediment, as it captures ageing that influences the distribution coefficient between sediment and overlying freshwater. For freshwater, a similar link is not easy to establish because measurement of (solid-phase) metal reactivity in the freshwater or coastal seawater is not so straightforward. A pragmatic solution would be to measure reactivity directly in the emission source and introduce a correction factor in the emission inventory assuming that this reactivity does not change over time. This assumption could be justified in freshwater, where fate factors are probably too small (in range of days to weeks) to allow for changes in reactivity to occur, unless very reactive (chemically) metal species are emitted. An alternative approach would be to determine (measure) what fraction of a metal is present in particulate forms in freshwater and coastal seawater and assume that this fraction is inert (Diamond et al. 2010). Implications of both approaches on the fate factor in freshwater or seawater need to be examined.

d. Link to inventory databases (needs for additional inventory features, needs for additional inventory flows, classification or differentiation etc.)

The use of generic (metal-specific) accessibility factors has no implication on the current inventory practice as metals can be reported according to the element and its oxidation state. If the emissions source-specific accessibility factors are used, however, inventory procedures for metal emissions should provide information about the metal emission source if that source is known. For soil, the classification of emission sources into a few archetypes based on their expected differences in metal accessibility may be used as guidance (Owsianiak et al. 2015). Indeed, chemical forms in emission archetypes originate from similar processes or are similar with regard to the composition of the matrix surrounding the metal in the emission, explaining statistically significant differences in accessibility between emission archetypes. In Owsianiak et al. (2015), the "airborne" archetype included emissions from smelters, metal refineries, factories, combustion of petrol, and unspecified atmospheric deposition. The "organic-related" archetype included direct application of biosolids, manure, compost, or wastewater irrigation. The "mining and industrial waste" archetype included emissions from mine spoils, mining-affected sediment, material containing metal ores, alluvial deposition, unspecified industrial waste, and technosols. Emissions from zinc oxide (isolated or in tire debris), mixed anthropogenic sources, unspecified anthropogenic sources, and dissolved metal forms of anthropogenic origin of emission (such as metal present as a co-contaminant in organic fertilizers, copper sulphate applied as a fungicide, or aqueous zinc dissolving from galvanized power lines) were included in the "other anthropogenic" archetype.

The link between inventory and impact assessment, addressing issues with handling group emissions in the (eco)toxicity context, is further detailed in the cross-cutting chapter (Chapter 2).

e. Roadmap for additional tests

Calculating characterisation factors using the recommended approaches requires following additional tests:

1. Test the reliability of correction factors for translating from various effect endpoints to chronic EC10-equivalents
2. Establish the link between P20-SSD based on chronic EC10-equivalents and potentially disappeared fraction of species
3. Evaluate the performance of various techniques to measure reactive fraction of metals in soil and freshwater sediment and derive accessibility factors
4. Test the influence of ageing time on metal accessibility in freshwater sediment
5. Improve the link between inventory and impact assessment for metals, which can exist in distinct chemical forms

f. Next foreseen steps

The next major steps within the coming 12 months–3 years are:

1. collate various databases, develop a procedure for curating effect data, and create an effect database in a reproducible, transparent, and expandable format;
2. collect physicochemical properties for substances of interest;
3. derive SSD curves and analyse patterns in the effect data;
4. calculate characterisation factors using recommended approaches; and
5. publish an article describing the relationship between chronic EC10-equivalents and PDF.

It should be realised that it is a substantial effort to collate and curate different databases and remove double entries. A pragmatic approach consists of bringing together the raw and/or curated databases, collate this data, and curate the net set that results. This database, constructed on the basis of published data, regulatory data (partly non-traceable according to common scientific principles), and data compilations curated by the respective database managers, would provide a pragmatic basis for deriving next-version effect factors.

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7.10 Appendix

7.10.1 Criteria of good practice and evaluation of existing approaches.

Table S7.1. Evaluation of new approaches to exposure factor of various organic compounds against generic criteria of good practice.

Criterion	Freshwater (Mehrkesh and Karunanithi 2016)	Freshwater (Morais et al. 2013)	Freshwater (Igos et al. 2014)
General 1: Number and types of substances covered	Ionic liquids (methylimidazolium- and 1-butylpyridinium-based)	Pharmaceuticals (Diclofenac, Ibuprofen, Atenolol, Carbamazepine, Bezafibrate, Diazepam, Fenofibrate, Mefenamic acid Phenazone, Atorvastatin, Clarithromycin Sulfamethazine, Cimetidine, Sulfathiazole, Hydrochlorothiazide)	Ionic and nonionic detergents (alcohols C11 eth- oxylated propoxylated; alcohols C8-C10 ethoxylated; Na-percarbonate; N,N0-ethylenebis[N-acety-lacetamide]: pentasodium triphosphate; polyethyl-ene glycol (PEG); silicic acid sodium salt; sodium carbonate; tetrasodium (1-hydroxyethylidene) bisphosphonate; acrylic/ sulphonic polymer; polymer acrylic/maleic)
Environmental mechanism 1: Exposure considers sorption to suspended matter: WELL/PARTIALLY/NO/NOT RELEVANT	WELL	WELL	WELL
Environmental mechanism 2: Exposure considers sorption to dissolved organic carbon: WELL/PARTIALLY/NO/NOT RELEVANT	WELL	WELL	WELL
Environmental mechanism 3: Exposure considers uptake by biota? YES/NO	YES	YES	YES
Environmental mechanism 4: Exposure considers solid-phase speciation (metals only): WELL/PARTIALLY/NO/NOT RELEVANT	NOT RELEVANT	NOT RELEVANT	NOT RELEVANT
Environmental mechanism 5: Exposure considers time-dependent changes in the solid-phase speciation (i.e., ageing and weathering mechanisms) (metals only): WELL/PARTIALLY/NO/NOT RELEVANT	NOT RELEVANT	NOT RELEVANT	NOT RELEVANT
Environmental mechanism 6: Exposure considers liquid-phase speciation (metals only): WELL/PARTIALLY/NO/NOT RELEVANT	NOT RELEVANT	NOT RELEVANT	NOT RELEVANT
Environmental mechanism 7: Exposure considers dissociation (organics acids and bases) or existence of a chemical in various forms (ionic liquids): WELL/PARTIALLY/NO/NOT RELEVANT	NO	YES	NO

Criterion	Freshwater (Mehrkesh and Karunanithi 2016)	Freshwater (Morais et al. 2013)	Freshwater (Igos et al. 2014)
Environmental mechanism 8: Exposure considers aggregation (nanoparticles): WELL/PARTIALLY/NO/NOT RELEVANT	NOT RELEVANT	NOT RELEVANT	NOT RELEVANT
Robustness and certainty 1: Peer review performed? YES/PARTIALLY/NO	YES	YES	YES
Robustness and certainty 2: Timeliness of model and data used (up-to-date knowledge): UP-TO-DATE, INTERMEDIARY, OUTDATED	UP-TO-DATE	UP-TO-DATE	UP-TO-DATE
Robustness and certainty 3: Contentious elements or limitation: NONE/LIST ANY	Ionic liquids treated as neutral entities, disregarding their ionic nature	NONE	Inorganic ingredients modelled by using only parameters required for organics
Robustness and certainty 4: Model evaluation: COMPREHENSIVE EMPIRICAL/ PARTIAL EMPIRICAL/MODEL COMPARISON/NONE	NONE	NONE	NONE
Robustness and certainty 5: Parameter uncertainty quantified: QUANTITATIVELY/ QUALITATIVELY/NONE	QUANTITATIVELY (A uniform distribution with variation of 1 order of magnitude in each direction was assigned to each model input parameter)	QUANTITATIVELY (Monte Carlo)	NONE
Robustness and certainty 6: Scenario and model uncertainty quantified/ addressed: QUANTITATIVELY/ QUALITATIVELY/NONE	NONE	NONE	NONE
Robustness and certainty 7: Spatial variability quantified/ addressed: QUANTITATIVELY/ QUALITATIVELY/NONE	NONE	NONE	NONE
Applicability 1: Implications for modelling fate factors: NONE/SOME; LIST ANY	NONE (XF can be directly combined with ff as done in the study)	NONE (XF can be directly combined with ff as done in the study)	NONE (XF can be directly combined with ff as done in the study)
Applicability 2: Implications for modelling effect factors: NONE/SOME; LIST ANY	NONE (XF can be directly combined with total dissoved based ef as done in the study)	NONE (XF can be directly combined with total dissoved based ef as done in the study)	NONE (XF can be directly combined with total dissoved based ef as done in the study)

Table S7.2. Evaluation of new approaches to exposure factor of nanoparticles against generic criteria of good practice.

Criterion	Freshwater (Eckelman et al. 2012)	Freshwater (Salieri et al. 2015)	Freshwater (Pu et al. 2016)	Freshwater (Deng et al. 2017)	Freshwater (Ettrup et al. 2017)
General 1: Number and types of substances covered	Nanoparticle (carbon nanotubes, CNT)	Nanoparticle (titanium dioxide, TiO_2)	Nanoparticle (copper, nano-Cu)	Nanoparticle (graphene oxide, GO)	Nanoparticle (titanium dioxide, TiO_2)
Environmental mechanism 1: Exposure considers sorption to suspended matter: WELL/PARTIALLY/NO/ NOT RELEVANT	WELL	NO (Precautionary approach applied; XF=1)	NO (XF=1 to avoid significant errors in ENPS fate predictions)	WELL	NO (Heteroagregated particles assumed bioavailable; XF=1)
Environmental mechanism 2: Exposure considers sorption to dissolved organic carbon: WELL/PARTIALLY/NO/ NOT RELEVANT	WELL	NO (Precautionary approach applied; XF=1)	NO (XF=1 to avoid significant errors in ENPS fate predictions)	NOT RELEVANT	NO (heteroagregated particles assumed bioavailable; XF=1)
Environmental mechanism 3: Exposure considers uptake by biota? YES/NO	YES	NO (Precautionary approach applied; XF=1)	NO (XF=1 to avoid significant errors in ENPS fate predictions)	YES	NO (heteroagregated particles assumed bioavailable; XF=1)
Environmental mechanism 4: Exposure considers solid-phase speciation (metals only): WELL/PARTIALLY/NO/NOT RELEVANT	NOT RELEVANT	NOT RELEVANT	NOT RELEVANT	NOT RELEVANT	NOT RELEVANT
Environmental mechanism 5: Exposure considers time-dependent changes in the solid-phase speciation (i.e., ageing and weathering mechanisms) (metals only): WELL/PARTIALLY/NO/ NOT RELEVANT	NOT RELEVANT	NOT RELEVANT	NOT RELEVANT	NOT RELEVANT	NOT RELEVANT
Environmental mechanism 6: Exposure considers liquid-phase speciation (metals only): WELL/PARTIALLY/NO/ NOT RELEVANT	NOT RELEVANT	NOT RELEVANT	NOT RELEVANT	NOT RELEVANT	NOT RELEVANT
Environmental mechanism 7: Exposure considers dissociation (organics acids and bases) or existence of a chemical in various forms (ionic liquids): WELL/PARTIALLY/NO/ NOT RELEVANT	NOT RELEVANT	NOT RELEVANT	NOT RELEVANT	NOT RELEVANT	NOT RELEVANT

Criterion	Freshwater (Eckelman et al. 2012)	Freshwater (Salieri et al. 2015)	Freshwater (Pu et al. 2016)	Freshwater (Deng et al. 2017)	Freshwater (Ettrup et al. 2017)
Environmental mechanism 8: Exposure considers aggregation (nanoparticles): WELL/PARTIALLY/NO/ NOT RELEVANT	NO	NO	NO	WELL	NO
Robustness and certainty 1: Peer review performed? YES/PARTIALLY/NO	YES	YES	YES	YES	YES
Robustness and certainty 2: Timeliness of model and data used (up-to-date knowledge): UP-TO-DATE, INTERMEDIARY, OUTDATED	UP-TO-DATE	UP-TO-DATE	UP-TO-DATE	UP-TO-DATE	UP-TO-DATE
Robustness and certainty 3: Contentious elements or limitation: NONE/LIST ANY	Nanoparticle treated as organic entity; aggregation not accounted for in calculation of XF (It was considered exogenously as removal mechanism in ff calcualation)	Free and aggregated particles assumed bioavailable	Free and aggregated particles assumed bioavailable	Free nanoparticle assumed bioavailable	Free and aggregated particles assumed bioavailable
Robustness and certainty 4: Model evaluation: COMPREHENSIVE EMPIRICAL/PARTIAL EMPIRICAL/MODEL COMPARISON/NONE	NONE	NONE	NONE	MODEL COMPARISON	MODEL COMPARISON
Robustness and certainty 5: Parameter uncertainty quantified: QUANTITATIVELY/ QUALITATIVELY/NONE	QUANTITATIVELY (A monte carlo analysis was performed within the usetox model, uniform distributions assumed)	NONE	NONE	QUANTITATIVELY	NONE
Robustness and certainty 6: Scenario and model uncertainty quantified/ addressed: QUANTITATIVELY/ QUALITATIVELY/NONE	QUANTITATIVELY (Realistic and worst case scenarios considered)	NONE	NONE	NONE	NONE
Robustness and certainty 7: Spatial variability quantified/addressed: QUANTITATIVELY/ QUALITATIVELY/NONE	NONE	NONE	NONE	NONE	NONE

Criterion	Freshwater (Eckelman et al. 2012)	Freshwater (Salieri et al. 2015)	Freshwater (Pu et al. 2016)	Freshwater (Deng et al. 2017)	Freshwater (Ettrup et al. 2017)
Applicability 1: Implications for modelling fate factors: NONE/SOME; LIST ANY	SOME; FF must consider aggregation	SOME; FF must consider aggregation	NONE (XF can be directly combined with FF as done in the study)	NONE (XF can be directly combined with FF as done in the study)	NONE (XF can be directly combined with FF as done in the study)
Applicability 2: Implications for modelling effect factors: NONE/SOME; LIST ANY	SOME; EF must consider aggregation	NONE (XF can be directly combined with total dissoved based EF (incl. Free and aggregated particles) as done in the study)	NONE (XF can be directly combined with total dissoved based EF (incl. Free and aggregated particles) as done in the study)	SOME; EF must be expressed as free nanoparticle form (not done in their study)	NONE (XF can be directly combined with total dissoved based EF (incl. Free and aggregated particles) as done in the study)

Table S7.3. Evaluation of new approaches to exposure factor of metallic elements against generic criteria of good practice.

Criterion	Soil (Owsianiak et al. 2013; Owsianiak et al. 2015)	Soil (Plouffe et al. 2015)	Marine (Dong et al. 2016)
General 1: Number and types of substances covered	Metallic elements (Cd, Co, Cu, Ni, Pb, Zn) emitted from various sources (spiked, airborne, organic-related, mining and industrial waste, other anthropogenic)	Metallic element (Zn)	Metallic elements (Cd, Cr[III], Co, Cu), Fe(III), Mn, Ni, Pb, and Zn)
Environmental mechanism 1: Exposure considers sorption to suspended matter: WELL/PARTIALLY/NO/ NOT RELEVANT	WELL	WELL	WELL
Environmental mechanism 2: Exposure considers sorption to dissolved organic carbon: WELL/PARTIALLY/NO/ NOT RELEVANT	WELL	WELL	WELL
Environmental mechanism 3: Exposure considers uptake by biota? YES/NO	NO	NO	NO
Environmental mechanism 4: Exposure considers solid-phase speciation (metals only): WELL/PARTIALLY/NO/ NOT RELEVANT	YES	NO	NO

Criterion	Soil	Soil	Marine
	(Owsianiak et al. 2013; Owsianiak et al. 2015)	(Plouffe et al. 2015)	(Dong et al. 2016)
Environmental mechanism 5: Exposure considers time-dependent changes in the solid-phase speciation (i.e., ageing and weathering mechanisms) (metals only): WELL/PARTIALLY/NO/NOT RELEVANT	WELL	NO	NO
Environmental mechanism 6: Exposure considers liquid-phase speciation (metals only): WELL/PARTIALLY/NO/ NOT RELEVANT	WELL (Cu, Ni), NOT STUDIED FOR Cd, Co, Pb, Zn)	WELL	WELL
Environmental mechanism 7: Exposure considers dissociation (organics acids and bases) or existence of a chemical in various forms (ionic liquids): WELL/PARTIALLY/NO/ NOT RELEVANT	NOT RELEVANT	NOT RELEVANT	NOT RELEVANT
Environmental mechanism 8: Exposure considers aggregation (nanoparticles): WELL/PARTIALLY/NO/NOT RELEVANT	NOT RELEVANT	NOT RELEVANT	NOT RELEVANT
Robustness and certainty 1: Peer review performed? YES/PARTIALLY/NO	YES	YES	YES
Robustness and certainty 2: Timeliness of model and data used (up-to-date knowledge): UP-TO-DATE, INTERMEDIARY, OUTDATED	UP-TO-DATE	UP-TO-DATE	UP-TO-DATE
Robustness and certainty 3: Contentious elements or limitation: NONE/LIST ANY	NONE	Conversion from exchangeable base cations to porewater dissolved based cations does not consider cation exchange equilibria	NONE
Robustness and certainty 4: Model evaluation: COMPREHENSIVE EMPIRICAL/PARTIAL EMPIRICAL/MODEL COMPARISON/NONE	PARTIAL EMPIRICAL	COMPREHENSIVE EMPIRICAL AND MODEL COMPARISON	NONE

Criterion	Soil (Owsianiak et al. 2013; Owsianiak et al. 2015)	Soil (Plouffe et al. 2015)	Marine (Dong et al. 2016)
Robustness and certainty 5: Parameter uncertainty quantified: QUANTITATIVELY/ QUALITATIVELY/NONE	NONE	NONE	NONE
Robustness and certainty 6: Scenario and model uncertainty quantified/ addressed: QUANTITATIVELY/ QUALITATIVELY/NONE	NONE	NONE	NONE
Robustness and certainty 7: Spatial variability quantified/addressed: QUANTITATIVELY/ QUALITATIVELY/NONE	QUANTITATIVE (XF calculated for global set of 760 soils)	QUANTITATIVE (XF calculated for 231 global soil archetypes)	QUANTITATIVE (XF calculated for 231 large marine ecosystems)
Applicability 1: Implications for modelling fate factors: NONE/SOME; LIST ANY	SOME FF must consider solid-phase reactivity of a metal	NONE	NONE (XF can be directly combined with ff as done in the study
Applicability 2: Implications for modelling effect factors: NONE/SOME; LIST ANY	SOME EF must be based on free ion	SOME EF must be based on "true solution" metal	SOME EF must be based on "truly dissolved" metal

Table S7.4. Evaluation of selected potential approaches to effect factor against generic criteria of good practice.

Criterion	HC50-EC50 (Hauschild et al. 2008a; Rosenbaum et al. 2008; 2011)	HC5-NOEC (European Commission 2003)	PNEC-NOEC (European Commission 2006; European Commission 2009)	Lowest validated endpoint (EC50, NOEC, or EC10) across at least 3 trophic levels (European Commission 2008)	Weighted average of lowest toxicity for 3 trophic levels (Finizio et al. 2001)
General characteristics					
Number and types of substances covered (e.g., NON-DISSOCIATING ORGANICS, DISSOCIATING ORGANICS, IONIC LIQUIDS, CATIONIC METALS, NANOPARTICLES, SUM EMISSIONS, OTHER-DESCRIBE)	Depending on available test data – in principle all	Depending on available test data – in principle all	Depending on available test data – in principle all	Depending on available test data – in principle all	Depending on available test data – in principle all
Marginal or average damage? The model based on a) average damage or b) on marginal increase in damage?	Average	Marginal	Not related to SSD	Relation to SSD unknown	Relation to SSD unknown

Criterion	HC50-EC50 (Hauschild et al. 2008a; Rosenbaum et al. 2008; 2011)	HC5-NOEC (European Commission 2003)	PNEC-NOEC (European Commission 2006; European Commission 2009)	Lowest validated endpoint (EC50, NOEC, or EC10) across at least 3 trophic levels (European Commission 2008)	Weighted average of lowest toxicity for 3 trophic levels (Finizio et al. 2001)
Value choices (List main value choices)					
LCA or risk assessment. The model based on a) best estimate or b) on safety factors/ precautionary hypotheses	LCA	ERA	ERA	HAZARD RANKING	HAZARD RANKING
Completeness of scope					
Geographical scope (Describe the overall geographical scope for which the models/ factors are determined [GLOBAL, SINGLE CONTINENT {list continent}, COUNTRY {list country}, OTHER-DESCRIBE])	Depending on available test data – in principle all	Depending on available test data – in principle all	Depending on available test data – in principle all	Depending on available test data – in principle all	Depending on available test data – in principle all
Compatibility					
Fit to overall LCA requirements (e.g., per functional unit impacts). The approach fits to overall LCA framework: WELL/ PARTIALLY/NO. List any restriction.		Doesn't support damage modelling (based on no effect concentrations)	Doesn't support damage modelling (based on no effect concentrations)	Quantitative relation to loss of species (damage indicator) not clear	Quantitative relation to loss of species (damage indicator) not clear
Environmental relevance					
Effects consider differences in ecotoxicity between different forms of a substance in the liquid phase. This mechanism is covered: WELL/ PARTIALLY/NO/NOT RELEVANT. List any restriction. Explain why not relevant.	Depending on available test data – in principle yes	Depending on available test data – in principle yes	Depending on available test data – in principle yes	Depending on available test data – in principle yes	Depending on available test data – in principle yes
Effects based on effect data for the compartment of interest. This mechanism is covered: WELL/PARTIALLY/NO. List any restriction.	Well	Well	Well	Well	Well
Effects based on chronic data. This mechanism is covered: WELL/PARTIALLY/NO. List any restriction.	Well	Well	Well	Well	Well

Criterion	HC50-EC50 (Hauschild et al. 2008a; Rosenbaum et al. 2008; 2011)	HC5-NOEC (European Commission 2003)	PNEC-NOEC (European Commission 2006; European Commission 2009)	Lowest validated endpoint (EC50, NOEC, or EC10) across at least 3 trophic levels (European Commission 2008)	Weighted average of lowest toxicity for 3 trophic levels (Finizio et al. 2001)
Effects consider competition from protons and/or base cations for uptake of a substance from the dissolved phase (metals only). This mechanism is covered: WELL/PARTIALLY/NO/ NOT RELEVANT. List any restriction. Explain why not relevant.	Only if ecotoxicity test data reflect BLM data	Only if ecotoxicity test data reflect BLM data	Only if ecotoxicity test data reflect BLM data	Only if ecotoxicity test data reflect BLM data	Only if ecotoxicity test data reflect BLM data
Effects consider biodiversity. This mechanism is covered: WELL/PARTIALLY/NO. List any restriction.	Predicts affected fraction of species and relates to disappeared fraction of species	Protects ecosystem, doesn't quantify biodiversity effects	Protects ecosystem, doesn't quantify biodiversity effects	Protects ecosystem, doesn't quantify biodiversity effects	Protects ecosystem, doesn't quantify biodiversity effects
Scientific robustness and certainty					
Peer review performed: YES/ PARTIALLY/NO	YES	YES	YES	PARTIALLY	PARTIALLY
Recognised/peer reviewed in process run by authoritative body? YES/PARTIALLY/ NO Describe review process and authoritative body	PARTIALLY	YES	YES	YES	NO
Timeliness of model and data used (up-to-date knowledge: UP-TO-DATE, INTERMEDIARY, OUTDATED	UP-TO-DATE	UP-TO-DATE	UP-TO-DATE/ INTERMEDIARY	INTERMEDIARY/ OUTDATED	INTERMEDIARY/ OUTDATED
Contentious elements or limitation. List any.	Unknown	Unknown	Unknown	Unknown	Equal weighting of species
Model evaluation: COMPREHENSIVE EMPIRICAL/PARTIAL EMPIRICAL/MODEL COMPARISON/NONE	MODEL COMPARISON	PARTIAL EMPIRICAL	MODEL COMPARISON	NONE	NONE
Parameter uncertainty quantified: QUANTITATIVELY/ QUALITATIVELY/NONE	QUANTITATIVELY	QUANTITATIVELY	NONE	NONE	NONE
Scenario and model uncertainty quantified/addressed: QUANTITATIVELY/ QUALITATIVELY/NO	QUANTITATIVELY	QUANTITATIVELY	QUALITATIVELY	NONE	NONE

Criterion	HC50-EC50 (Hauschild et al. 2008a; Rosenbaum et al. 2008; 2011)	HC5-NOEC (European Commission 2003)	PNEC-NOEC (European Commission 2006; European Commission 2009)	Lowest validated endpoint (EC50, NOEC, or EC10) across at least 3 trophic levels (European Commission 2008)	Weighted average of lowest toxicity for 3 trophic levels (Finizio et al. 2001)
Applicability					
Implications for modelling fate factors. List any implications.	NONE	NONE	NONE	NONE	NONE
Implications for modelling exposure factors. List any implications.	Consideration of bioconcentration when acute test data is applied?	Consideration of bioconcentration when acute test data is applied?	Consideration of bioconcentration when acute test data is applied?	Consideration of bioconcentration when acute test data is applied?	Consideration of bioconcentration when acute test data is applied?

7.10.2 Interpretation of fate factor

Recall, that a change in steady-state substance amount in the water column that results from a unit change in the emission flow rate is mathematically equivalent to the overall cumulative amount from a pulse emission, accounting for the environmental residence time of the substance (Heijungs 1995) (Figure S7.1). For example, USEtox predicts that mass of benzaldehyde (CAS 100-52-7) in coastal freshwater at steady state is equal to 16.2 kg for a unit emission flow rate (1 kg/day) to coastal freshwater, resulting in a fate factor in this compartment equal to 16.2 days (Fig. S7.1a). For the reasons given in section 7.4.4, the area below the curve in Fig. S7.1b, showing mass decrease due to pulse emission of 1 kg, is also equal to 16.2 kg. This implies that both short-term and long-term impacts are considered (with equal weight), even if infinite time horizons are used to calculate fate factors and resulting characterisation factors in line with not applying any weighting for current versus future impacts.

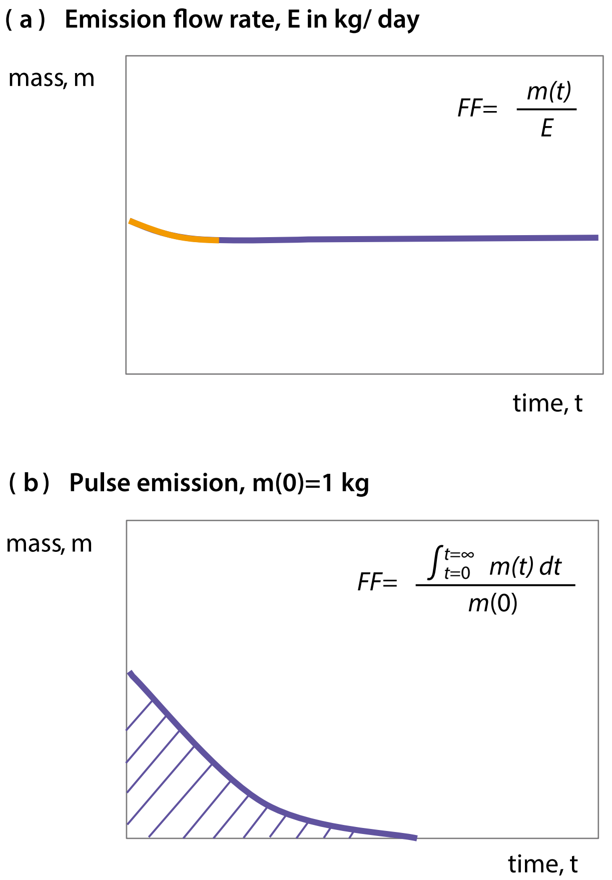

Figure S7.1: Interpretation of a fate factor, FF. Orange line represents short-term mass increase resulting from emission (input for short-term impacts). Dividing steady-state mass increase m [kg] at time t by emission flow rate E=1 [kg/day] results in FF [kg per kg/day] – this is how fate factor is calculated in current LCIA multimedia fate models (a). For a model where steady state mass increase is a linear function of emission flow rate, this is mathematically equivalent to integrating mass over time for a unit (1 kg) pulse emission (b).

8. Integration and Synthesis

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8.1 The SETAC Pellston Workshop process

This guidance document is a result of intensive efforts by an international group of experts to identify consensus on selected environmental impact category indicators, on the overall life cycle impact assessment framework, and on cross-cutting issues. The careful evaluation of existing environmental impact category indicators, representing human toxicity, ecotoxicity, acidification and eutrophication, soil quality, and ecosystem services impacts caused by land use and mineral primary resources was the subject of a focused analysis process. The findings and recommendations on these indicators and on the cross-cutting issues are presented in the previous chapters. These recommendations have been characterised by their level of maturity and degree of reliance and confidence. Those characterisations need be taken into account when applying the recommended indicators and help to define and prioritise further developments of indicators or aspects of the assessment framework.

The topics addressed are not stand-alone and have the potential to be integrated into the broader picture of life cycle impact assessment (LCIA). This chapter provides such an integration and synthesis, as well as key messages of the topics covered. One element of this integration encompasses the cross-cutting issues to which all recommended environmental impact category indicators refer. They are complementary to the cross-cutting issues and recommendations made in Volume 1 of these Guidelines (Frischknecht and Jolliet 2016). Key aspects of the specific indicators and their related recommendations are covered in the subsequent sections of this chapter (after the section on cross-cutting issues).

Developing further environmental impact category indicators systematically, in line with the overall framework, and adhering to the recommendations related to cross-cutting issues is highly important and strongly recommended by the guidance principles. This will foster the application and acceptance of life cycle-based environmental indicators and facilitate the development of comprehensive and consistent LCIA methods.

8.2 Cross-cutting issues

LCA encompasses both an assessment framework, assessment steps, and a suite of indicators. Both the current LCA methods, as well as future method developments, resulting from scientific innovations imply that substantial attention needs to be paid to harmonisation and cross-cutting issues. There are multiple cross-cutting issues that need harmonisation, and the task force moved a step forward in that respect. The ultimate goal is that all new developments can be integrated into LCIA in a consistent and compatible way and that the connection to life cycle inventory (LCI) is harmonised.

The task force on cross-cutting issues have investigated several topics, four of which were discussed at the Pellston Workshop: uncertainty assessment and management, instrumental values framework, vulnerability aspects related to ecosystem quality, and a harmonised connection between LCI and LCIA. In Chapter 2, a series of short- and long-term recommendations for the four topics are listed, mostly for method developers, but also for practitioners and software developers. We would like to highlight the following short-term recommendations:

- It is strongly recommended to interpret and report uncertainties for all relevant uncertainty types, as well as for the associated variability. This is strongly recommended for both practitioners and method developers and should be done using the recommended tiered approach from Chapter 2.
- We recommend mapping the ecosystem services according to existing classification systems and identifying the connections between life cycle inventory analysis (LCI) and/or LCIA with the mapped ecosystem services. Outlining the detailed cause-effect chains that capture all ecosystems services is strongly recommended as a follow-up step.
- For ecosystem services, we strongly recommend avoiding double counting. However, we highlight that one ecosystem service may contribute to several areas of protection (AoPs) (human health, ecosystem quality, natural resources, ecosystem services, socioeconomic systems, natural or cultural heritage), as exemplified in Chapter 2.

- We strongly recommend addressing vulnerability consistently across all impact categories feeding into the AoP ecosystems quality and constructing vulnerability scores in a way that allows aggregation of indicator scores across all impact categories at the end of the impact pathway.
- We interim recommend that practitioners use the already published vulnerability scores, bearing in mind that these currently have limitations when it comes to the coverage of impact categories and taxonomic groups.
- We strongly recommend that all stakeholders support and develop a common reference nomenclature and classification system for specifying the name of elementary flows, classifications (e.g., to distinguish chemical classes and compartments), and associated properties (e.g., technical, chemical, or economic flow properties). Both nomenclature and classification systems have evolving natures, which in principle can be developed at the lowest level of detail, so that the differentiation within the classifications can be seen as an aggregate of two or more of this evolving base nomenclature (e.g., indoor air emissions consists of household indoor and industrial indoor emissions). Until such a common unique nomenclature system is developed, we recommend following the nomenclature systems developed by ecospold or ILCD system (EC 2010), or at a minimum, providing clear descriptions of the used nomenclature.

Additionally, a number of future developments in relation to long-term recommendations are outlined for each investigated topic in Chapter 2. These are issues where more research is needed to arrive at final recommendations. We highlight the following topics for future research:

- We recommend that software developers enable quantitative uncertainty assessment across LCI and LCIA, including in cases of spatially (and temporally) differentiated assessments.
- We recommend that LCIA method developers investigate the suitability of a Pedigree matrix for LCIA as well as other uncertainty aspects, such as border issues, correlation uncertainty within LCI and LCIA, or the uncertainty normalisation to enable comparability of uncertainty metrics.
- We recommend that method developers in LCI and LCIA develop an operational framework for ecosystem services, including different temporal and spatial scales.
- We recommend that LCIA method developers continue the efforts to include ecological vulnerability in general and operational vulnerability scores, and to keep on exploring additional indicators (such as functional diversity) that may add to the quantification of damages.

Across all the recommendations, future developments, and harmonisation issues, we concluded that transparent reporting is a key aspect to improving the utility of LCA outcomes for practical decision-making. We therefore urge all practitioners and method and software developers to follow the guidelines for transparent reporting made in the previous Pellston Workshop report.

8.3 Human toxicity

For a human toxicity metric, where LCIA is seeking a quantitative estimate of the capacity to cause harm, a goal is driven by the need for making substance and product-service system comparisons in LCA. Current practice for providing human toxicity characterisation factors is incorporated in the USEtox model and its associated databases. USEtox is meant to reflect mature science. However, the current toxicity characterisation framework in LCIA has limitations that called for further improvement based on new scientific findings. Significant among these improvements are:

1. addressing spatiotemporal and population-level resolution to estimate impact potential;
2. addressing chemical substances in consumer products and in occupational settings, and adding related human exposure pathways that are currently missing;
3. extending the limited coverage in available dose-response data and models; and
4. improving the coverage and quality in databases on substance physicochemical properties and toxicity information.

We considered the consensus-based framework of Rosenbaum et al. (2008) as a starting point for assessing human toxicity impacts in LCIA. In order to combine exposure pathways in the near-field (consumer and occupational environments) with existing far field (outdoor environment) processes, we reviewed a number of available exposure-model options and identified an approach that considers human exposures during and after product use, exposure of bystanders, and occupational exposure pathways. We recommend consistent mass-balance models to link near-field environments to human receptors following the approach of Fantke et al. (2016).

The effect factors for human toxicity are indicators that are derived from measures of toxic potential used in the chemical risk assessment arena. Such indicators are derived directly from information on chemical potency in humans where available. However, in most cases, human data are not available such that indicators of human toxicity are often derived from animal experiments or, when such data are missing, from quantitative structure-activity relationships (QSAR) or other sources. These indicators are derived both for carcinogenic and non-carcinogenic toxicity endpoints, depending on the chemical-specific data available. This effect factor is combined with exposure and damage factors to provide the human toxicity characterisation factor. Damage factors translate an estimated human response to units of disability-adjusted life years (DALYs). In our revised approach, the selection of toxicity data, extrapolation of these data to derive effect factors for non-cancer endpoints, and the estimation of damage factors associated with non-cancer responses are refined.

In cases where the impact of uncertainty on a chemical's DALY contribution is found to be consequential, the best approach to characterise the impact is to conduct sensitivity analysis, repeating the calculations with alternative values of the uncertain elements that deemed to be supportable in view of the available information.

Recommended steps include expansion and full implementation of the matrix framework of Fantke et al. (2016) to address product-related exposures and calculation of both intake fractions and product intake fractions, allowing flexibility to introduce additional exposure models into the matrix framework. Recommendations for the dose-response side include a) implementation of the WHO/IPCS extrapolation approaches for non-cancer dose-response for chemicals with toxicity data available from a range of data sources, and b) refinement and updating of severity factors address developmental toxicity separately and to reflect current Global Disease Burden statistics. Finally, clear delineations of model applicability domains and recommendations on uncertainty, variability, and best practices for interpretation of outcomes of modelling are recommended.

8.4 Ecotoxicity

We derived a total of 19 specific recommendations, grouped around four major topics, with the ambition to update current LCIA practice in characterisation modelling of ecotoxicity while considering developments in science and availability of data.

The first group of recommendations addressed the relevance and feasibility of adding additional compartments and impact pathways into LCIA. The outcome was a recommendation to include effects of chemical substances on organisms living in coastal waters, soil, and freshwater sediment in LCIA, going beyond just freshwater. In absence of effect data for organisms specific to the compartment of interest, we suggest using extrapolation procedures from freshwater organisms. In this context, we formulated a specific overarching recommendation, to consider specific characteristics of chemicals, organisms, and compartments during the calculation of effect factors. This overarching recommendation could imply deviations from the suggested extrapolation procedures. This overarching recommendation is a consequence of the huge variety of chemicals, compartments, and organisms to be considered. Overall, addition of these compartments should contribute to a better representation of the total damage on ecosystems and should contribute to identification of substances with the largest potential to cause harm in the respective compartment.

The second major group of recommendations addresses selection of an ecotoxicity indicator and its relation to damage. The major recommendation here is to base effect modelling on a concentration domain of the SSD curve that is close to the domain of environmental concentrations. A 20th percentile was chosen as working point on an SSD curve, which is derived from chronic EC10-equivalents, comprising the chronic endpoints: No Observed Effect Concentration (NOEC); Lowest Observed Effect Concentration (LOEC); No-Observable Adverse Effect Level (NOAEL); Maximum Acceptable Toxicant Concentration (MATC); Effect Dose inducing a 50% response over background (EC50); and chronic Effect Concentration affecting x% of individuals above background (ECx); where x is between 1 and 20, adjusted by appropriate correction factors. In addition to being closer to environmentally relevant concentrations, selection of EC10-equivalents is also driven by availability of effect data, as the number of ecotoxicological effect data that are close to EC10 (like NOEC, LOEC) is larger compared with chronic EC50 values. Furthermore chronic EC50 values are not expected to be generated to a large extent in the future. Overall, the recommended ecotoxicity indicator is expected to reduce the risk that potentially relevant information is lost about particularly toxic (or particularly nontoxic) substances at environmentally relevant levels of pressure on ecosystems. A recommendation was also made to base damage on potentially disappeared fraction (PDF) of species, which implies that the link between chronic EC10-equivalents and the PDF must be established. To ensure transparency and allow for the controlled updating of ecotoxicity indicators, data used to calculate effect factors must have a traceable origin.

The third group of recommendations addresses issues associated with exposure modelling. To harmonise exposure modelling across compartments and to make the match between exposure factors and effect factors more consistent, we recommend disregarding bioaccumulation as the removal mechanism when calculating exposure factors. Implementation of this recommendation in practice will increase exposure factor for lipophilic substances. For metals, it was further recommended to consider liquid-phase speciation of metals in the compartment of interest, and furthermore, it was recommended to consider solid-phase reactivity (accessibility) as influenced by ageing and weathering mechanisms of a metal in soil and freshwater sediment. Consideration of speciation requires that effect factors are based on bioavailable concentrations. Free ion activity models are recommended for use to base effect factors on bioavailable concentrations. This choice was made to allow for unbiased ranking of those metals for which free ion is the dominant toxic metal form.

Finally, we made several recommendations that addressed issues associated with the interpretation of ecotoxicity characterisation factors and the presentation of resulting impact scores. Considering large variability in characterisation factors (which vary by several orders of magnitude) and their uncertainties (which vary 2 to 3 orders of magnitude), we recommend presenting impact scores on a log10-scale, separately for organic and inorganic compounds (including metals) while keeping them on the same (log10-transformed) scale. Moreover, we recommend stressing that ecotoxicity impact scores represent time- and space integrated potential (not actual) ecotoxic impact on receiving ecosystems when interpreting results. Our interim recommendation is to use the comparative toxic unit as unit of impact score.

The strength of the aforementioned recommendations ranges from interim to strong. Nevertheless, they all aim to represent stable science – science that is stable today and will remain stable in the future, irrespective of how science develops. Implementation of the recommendations in practice will allow for the harmonised assessment of chemical emissions in LCIA, particularly in product environmental footprint (PEF) studies.

8.5 Acidification and eutrophication

Despite substantial recent efforts to capture the effects of acidification and eutrophication in LCA, no clear consensus exists on the use of a specific impact indicator, and many LCA methods that do not account for fate and lack effect modelling are still in use. This variability in modelling approaches limits the comparability of results from different studies. There is a need to identify and achieve consensus on scientific approaches that advance beyond these basic approaches specifically, this group considered issues related to fate modelling, limiting nutrients, effect curve modelling, biological oxygen demand (BOD) and chemical oxygen demand (COD), and aggregation. Taken together, these recommendations represent an improvement for acidification and eutrophication modelling in LCIA. Recommended approaches are commensurable with other ecosystem impacts, such as ecotoxicity or responses to land use, to (ideally) allow for comparison of ecosystem damage resulting from different stressors.

We began our work with a review of existing LCA models for acidification and eutrophication. Given the spatial variability associated with these impact pathways, we focused on models with global applicability and spatially resolved modelling. The freshwater phosphorus model of Helmes et al. (2012), the atmospheric model for terrestrial acidification of Roy et al (2012a), and the aquatic nitrogen transport model of Cosme et al. (2017) represent a set of spatially differentiated, globally applicable fate models. While these are based on a variety of underlying models, ranging from empirical steady-state to reaction-driven dynamic models, they identify important geographic differences and were judged to provide valuable insight relative to other LCA models. For effect modelling of eutrophication, typical effect factors are based on stoichiometry of oceanic phytoplankton (the Redfield ratio), and therefore we recommend the empirically based, globally-derived effect factors of Azevedo et al. (2013a), which bring an important degree of sophistication to effect modeling. A similar recommendation is made for terrestrial acidification, using spatial soil models and global effect data (Roy et al. 2012b, Azevedo et al. 2013b). For marine eutrophication, the group suggests further research before the recommendation of an endpoint characterisation factor.

The group identified a number of short and long-term steps for future research. Across impact categories and spanning the cause-effect chain from fate to effect, the group recommends further research; for example, for fate, a comprehensive model should consider background concentrations of relevant species in receiving compartment (e.g., soils, freshwater, or marine waters), as has been accomplished with the GEOS-Chem model used for acidification. Such modelling would be a precursor towards a eutrophication model that accounts for possible co-limitation by phosphorus and nitrogen. At present, the inclusion of BOD/COD in LCA models has been based on stoichiometric equivalency factors; future modelling can more accurately capture the mechanisms associated with these substances. For effect, empirical data are used to build a species assemblage curve that serves as a dose-response function. The selection of a working point on the curve has often been a default; the group recommends harmonising the working point with other impact categories, and also recommends the provision of both marginal and average effect factors. Finally, because eutrophication and acidification are often associated with specific industries, such as agriculture, the group recommends that aggregated characterisation factors be provided based on such industries, and also at a population-weighted level, such that practitioners may choose amongst appropriate factors. The group also found the spatial and temporal variability of agricultural practices to be of utmost importance. While these can all be captured in an LCIA model, the group provided a tiered approach for estimating inventory emissions of nutrients in a variety of settings.

8.6 Soil quality and ecosystem services impacts caused by land use

Land use and land use change (LULUC) are key human stressors that can affect soil quality, e.g., by modifying physical, chemical, and biological properties of soil through agriculture and forestry, by altering the rate of soil production and/or removal, and/or sealing it through urbanisation and infrastructure. High quality functional soil is important for the supply of ecosystem services, such as provisioning biomass, collecting and cleaning freshwater, and absorbing and storing carbon.

A wide range of LCIA models were assessed by Vidal Legaz et al. (2017), and a subset of only those that are those currently available and operational were further assessed by the taskforce. These focus on soil organic carbon, biotic production, erosion, groundwater regeneration, mechanical filtration, and water infiltration capacity.

The change in soil organic carbon stock (ΔSOC, or SOC deficit, measured in kg SOC x year) was chosen as the indicator of soil quality, as it is an integrative indicator of soil functions being strongly linked to carbon transformations and soil structure maintenance, and linked to groundwater regeneration, mechanical filtration, and water infiltration capacity. The method by Brandão and Milà i Canals (2013) has been recommended (ad interim, pending some additional factors to better represent forest production and perennial agriculture, which should be available by the time the report is published). A suggestion has also been made to update the reference stock of SOC to calculate the CFs with the most up-to-date global database on SOC, recently published by FAO (2018).

While there is a link between SOC and erosion, there are some other much more important factors affecting erosion, such as water erosion. Therefore, a separate indicator, soil loss based on the revised universal soil loss equation (RUSLE), as implemented by Bos et al. (2016) with some modification, has been recommended ad interim to address soil erosion impacts.

We recommend that both of these CFs be applied in background database at the national level where the country is known (and for states for large nations crossing climate regions, where possible), otherwise at the global level. In the foreground, it is suggested that the specific soil type or the ecoregion level where the activity takes place is used. These factors are published alongside the global and national average data.

The aim in the future is to link the SOC and soil loss indicators to damage categories including human health, ecosystem quality, and natural resources (for soil loss). There are also developments underway to provide a more integrated assessment of soil quality based on empirical analyses of the multiple factors affecting the overall performance of the soil and expressing it in a soil quality index (SQI).

8.7 Natural resources (mineral primary resources)

Numerous impact assessment methods are available to assess different aspects of resource use and model different impact pathways leading to different LCIA results. In order to reach consensus on what should be protected with regard to resource in LCA, the safeguard subject and the impacts to be modelled have been defined as follows:

"Within the AoP 'natural resources,' the safeguard subject for 'mineral resources' is the potential to make use of the value resources, as embedded in a natural or anthropogenic stock, can hold for humans in the technosphere. The damage is quantified as the reduction or loss of this potential caused by human activity. Mineral resources are chemical elements (e.g., copper) or minerals (e.g., gypsum) or aggregates (e.g., sand)."

In a comprehensive literature review, 29 LCIA methods have been identified and grouped into four categories depending on the impact pathway modelled (depletion, future efforts, thermodynamic accounting, and supply risk methods). Subsequently, the methods have been discussed, analysed by means of an evaluation scheme, and applied in a case study of electric vehicles. The questions intended to be answered by these methods have been formulated and their relation to the safeguard subject has been described. At the Pellston workshop, we established a list of main questions that LC(S)A practitioners are interested in and assigned methods to these questions. As shown in the following table, these questions

Table 8.1. Questions related to the impacts of mineral resource use and matching recommended methods including the level of recommendation. Colours of the questions indicate the link of the question to the four method categories defined in Figure 5.2 green – depletion methods, yellow – future efforts methods, orange – thermodynamic accounting methods, blue – supply risk methods.

How can I quantify the relative…

...changing opportunities of future generations to use mineral resources due to a current mineral resource use? (inside-out)					**….potential mineral resource availability issues for a product system? (outside-in)**	
...contribution of a product system to the depletion of mineral resources?	...contribution of a product system to changing mineral resource quality?	...consequences of the contribution of a product system to changing mineral resource quality?	...(economic) externalities of mineral resource use?	…impacts of mineral resource use based on thermo-dynamics?	...potential availability issues for a product system related to mid-term physico-economic scarcity of mineral resources?	...potential accessibility issues for a product system related to short-term geopolitcal and socio-economic aspects?
ADP$_{\text{ultimate reserves}}$	Ore Grade Decrease	SOP	LIME2 (endpoint)	CEENE	ADP$_{\text{economic reserves}}$	ESSENZ
ADP$_{\text{reserve base}}$		ORI	Future Welfare Loss*	CExD	ADP$_{\text{reserve base}}$	GeoPolRisk
ADP$_{\text{economic reserves}}$		Eco-Indicator 99		TR	Eco-sWcarcity	ESP
Eco-scarcity		Impact 2002+		SED	AADP	
AADP		Stepwise 2006			AADP (update)	
AADP (update)		ReCiPe 2008			EDIP 97	
EDIP 97		SCP			EDIP 2003	
EDIP 2003		EPS			LIME2$_{\text{midpoint}}$	
LIME2$_{\text{midpoint}}$		TR-ERC				**Interim recommended**
Recommended		**Interim recommended**	**Interim recommended**	**Interim recommended**	**Suggested**	**Suggested**

Abbreveations: ADP: Abiotic Depletion Potential, AADP: Anthropogenic stock extended Abiotic Depletion Potential, ORI: Ore Requirement Indicator, SOP: Surplus Ore Potential, SCP: Surplus Cost Potential, TR: Thermodynamic Rarity, TR-ERC: Thermodynamic Rarity - Exergy Replacement Cost, CExD: Cumulative Exergy Demand, CEENE: Cumulative Exergy Extraction from the Natural Environment, SED: Solar Energy Demand, ESP: Economic Scarcity Potential, ESSENZ: Integrated Method to Assess Resource Efficiency, GeoPolRisk: Geopolitical Supply Risk

* The Future Welfare Loss method was not published at the time of the Pellston Workshop and, thus, could not be recommended. However, it models a relevant complementary impact pathway to the one described by LIME2 (endpoint) and this was discussed in detail prior to the workshop within the task force.

either address the impacts of a product system's resource use on the opportunities of future generations to use resources (inside-out) or resource availability for a product system (outside-in). We recommend using the inside-out-related questions within environmental LCA and the outside-in-related questions within broader life cycle-based approaches, such as life cycle sustainability assessment (LCSA). The most appropriate methods for answering the specific questions have been recommended considering their (a) modelling approach; (b) cause-effect pathway; (c) data used; and (d) coverage of CFs. Limitations of the recommended methods were addressed to the level of recommendation (e.g., interim recommendation).

For future method development we recommend (a) considering anthropogenic stocks in addition to natural stocks, (b) updating and increasing the number of CFs, (c) promoting LCA software implementation, and (d) quantifying uncertainties. In order to fully address the safeguard subject, we strongly recommend defining dissipative resource use (e.g., by specifying economic and technological thresholds) and implementing it into characterisation models.

Table 8.2. Characteristics of the environmental life cycle impact category indicators recommended, their domain of applicability and the level of recommendation

Impact category and subcategory	Cause-effect description	Indicator retained - Position in the cause effect chain Metric Unit	Factors of influence- Considered, spatial resolution Archetypes Time horizon	Key references	Domain of applicability	Level of recommendation
Human toxicity						
Consumer exposure	Chemical in product application – near-/far-field fate and human exposure	Product intake fraction (exposure level) kg intake per kg in product	Chemical mass in product, product archetypes, exposure dynamics considered	Metric: Jolliet et al. 2015; Framework: Fantke et al. 2016; Models: Huang et al. 2017	Different product categories; local to global scenarios	Recommended
Cancer effects	Carcinogenic effects in humans	TD50 as reference point; Midpoint: cases/kg intake Endpoint: DALY/kg intake	Cancer potency data; route-to-route extrapolation	Data: Gold 2011; Approach: Crettaz et al. 2002; Model: Rosenbaum et al. 2011	Generic/default	Recommended
Non-cancer effects	Developmental and other non-cancer effects in humans	ED10 as reference point; Midpoint: cases/kg intake Endpoint: DALY/kg intake	Non-cancer animal effect data; route-to-route extrapolation	Approach: WHO 2014; Framework: Chiu et al. 2015; Data and model: Chiu et al. 2018	Generic/default; for severity: regions/countries	Recommended
Ecotoxicity						
Freshwater ecotoxicity	From emission of chemical substances to potentially affected fraction of species (PAF)	HC50-EC10 equivalent Midpoint: CTUe/kg Endpoint: not available (link between EC10eq and PDF is missing)		Model: Rosenbaum et al. 2011 as starting point	Generic to regional	From recommended to strong, depending on specific recommendation underlying the indicators

Impact category and subcategory	Cause-effect description	Indicator retained - Position in the cause effect chain Metric Unit	Factors of influence- Considered, spatial resolution Archetypes Time horizon	Key references	Domain of applicability	Level of recommendation
Coastal water ecotoxicity	From emission of chemical substances to potentially affected fraction of species (PAF)	HC50-EC10 equivalent Midpoint: CTUe/kg Endpoint: not available (link between EC10eq and PDF is missing)	Extrapolation from freshwater effect data	Model: Rosenbaum et al. 2011 as starting point Framework (metals): Dong et al. 2016	Generic to regional	From recommended to strong, depending on specific recommendation underlying the indicators
Terrestrial ecotoxicity	From emission of chemical substances to potentially affected fraction of species (PAF)	Midpoint: CTUe/kg Endpoint: not available (link between EC10eq and PDF is needed to derive endpoint indicator)	Extrapolation from freshwater effect data	Model: Rosenbaum et al. 2011 as starting point; Framework (metals): Owsianiak et al. 2013; 2015	Generic to regional	From recommended to strong, depending on specific recommendation underlying the indicators
Freshwater sediment ecotoxicity	From emission of chemical substances to potentially affected fraction of species (PAF)	HC50-EC10 equivalent Midpoint: CTUe/kgEndpoint: not available (link between EC10eq and PDF is missing)	Extrapolation from freshwater effect data	Model: Rosenbaum et al. 2011 as starting point	Generic to regional	From interim to strong, depending on specific recommendation underlying the indicators
Acidification & Eutrophication						
Freshwater Eutrophication	P emissions to freshwater ➞ P increases in water ➞ PDF	P equivalent PDF	Fate: 0.5 x 0.5 degree, annual Effect: freshwater types + climate, autotrophs – heterotrophs	Fate: Helmes et al. 2012 Effect: Azevedo et al. 2013a	Local ➞ global	Recommended Recommended*
Marine Eutrophication	N emissions to soil, freshwater, and marine ➞ N is coastal surface ➞ primary production & respiration in benthic layer ➞ PDF	N eq PDF	Fate: river basins, annual Effect: 6 benthic taxonomic groups and 5 climate zones	Fate: Cosme et al. 2017 Exposure: Cosme et al. 2015 Effect: Cosme and Hauschild 2016	Local ➞ global	Recommended Suggested*
Terrestrial Acidification	NH3/NOx/SO2 emissions ➞ deposition ➞ pH change ➞ PDF	SO_2 eq PDF	Fate: 2x2.5 degree, annual Effect: vascular plants across 13 biomes	Fate: Roy et al. 2012b Effect: Azevedo et al. 2013b	Local ➞ global	Recommended Recommended

Impact category and subcategory	Cause-effect description	Indicator retained - Position in the cause effect chain Metric Unit	Factors of influence- Considered, spatial resolution Archetypes Time horizon	Key references	Domain of applicability	Level of recommendation
Impacts on soil quality and ecosystem services						
SOC deficit potential	Change is soil carbon formation due to land occup./ trans. and management in non-natural state.	Kg C Deficit	Native scale: Global, national and state level based on biomes	Brandão and Milà i Canals 2013	Biomes – mapped to national and/or sub-national for larger countries	Interim recommendation based on increased land use classes being defined
Soil erosion potential	Change is water erosion due to land occup./ trans. and management in non-natural state.	kg soil eroded	Native scale: Global, national and state level based on eco-regions	Bos et al. 2016	Ecoregions – to national and/or sub-national for larger countries	Suggested
Mineral primary resources						
ADP	Depletion of ultimate reserves	Abiotic Depletion Potential$_{\text{ultimate reserves}}$ kg Sb-eq	Global-Long-term (centuries)	Guinée and Heijungs 1995; Van Oers and Guinée 2016; CML 2016	Impacts on future generations: Quantification of the contribution of a product system to the depletion of resources	Recommended
SOP	Additional ore requirements of future extraction	Surplus Ore Potential kg Cu-eq/kg ore	Global-Long-term (centuries)	Vieira et al. 2016a; Vieira et al. 2016b	Impacts on future generations: Quantification of the contribution of a product system to changing resource quality	Interim recommended
LIME2	Economic externalities caused by resource use	User cost Yen	Global-Long-term (centuries)	Itsubo and Inaba 2014	Impacts on future generations: Quantification of the (economic) externalities of resource use	Interim recommended
CEENE	Valuing resources exergy terms	Cumulative Exergy Extraction from the Natural Environment MJ_{exergy}	Global-Short-term (current change)	Dewulf et al. 2007; Alvarenga et al. 2013; Taelman et al. 2014	Impacts on future generations: Quantification of the mineral resource use based on thermodynamics	Interim recommended
ADP	Resource scarcity with regard to economic reserves	Abiotic Depletion Potential$_{\text{economic reserves}}$ kg Sb-eq	Global-Mid-term (a few decades)	CML 2016	Resource availability: Quantification of potential resource availability issues for a product system related to physico-economic resource scarcity	Suggested

Impact category and subcategory	Cause-effect description	Indicator retained - Position in the cause effect chain Metric Unit	Factors of influence-Considered, spatial resolution Archetypes Time horizon	Key references	Domain of applicability	Level of recommendation
ESSENZ	Geopolitical and socio-economic supply risks	Set of 11 supply constraints (country concentration of reserves and mine production, price variation, co-production, political stability, demand growth, feasibility of exploration projects, company concentration, primary material use, mining capacity, trade barriers)	Global-Short-term (current change)	Bach et al. 2016	Resource availability: Quantification of potential resource availability issues for a product system related to short-term geopolitical and socio-economic aspects	Interim recommended
GeoPolRisk	Geopolitical and socio-economic supply risks	Political stability and country concentration	Country-Short-term (current change)	Cimprich et al. 2017; Helbig et al. 2016; Gemechu et al. 2015	Impacts on future generations: Quantification of the contribution of a product system to the depletion of resources	Recommended

* Strong recommendation for further, location-specific case studies

8.8 Vision and roadmap(s)

The work and discussions before and during the Pellston Workshop resulted in relevant recommendations in the five topical areas human toxicity, ecotoxicity, acidification and eutrophication, soil quality and its impact on ecosystem services, and mineral resources, as well as with regard to cross-cutting issues.

The characterisation factors and impact category indicators recommended include the latest findings from topical research and consensus built for that. The recommendations clearly go beyond current practices in the respective subjects. The levels of recommendation show the variable maturity of the indicators (see Table 1). At the same time, care has been taken to ensure immediate applicability in current LCA environments as far as possible.

This workshop format promoted progress in science, while fostering a community of teams and organisations to maintain the consensus indicators and characterisation factors. This community should take care to build capacity, establish recommendations on the proper use and interpretation of the environmental indicators developed, and co-ordinate potential future updates and developments. The community may grow when launching consensus-finding processes for additional environmental impacts caused by nutrition or noise.

Spatial resolution is an issue common to several of the topical areas, i.e., ecotoxicity, human toxicity, acidification and eutrophication, as well as soil quality. All groups agreed on providing characterisation factors on the native scale (like grid cells for acidification and eutrophication), as well as on more aggregated levels such as river basins, countries, continents, and the globe, or archetypical situations such as indoor or outdoor and rural or urban exposures.

While the need for spatial differentiation is acknowledged in decision situations dealing with the foreground system, it is a challenge to underpin spatially explicit product LCA models with the LCI data and information required. Thus, it is an important task to derive smart and parsimonious approaches from the knowledge gained in LCIA research projects in which a high geographic resolution is applied.

The United Nations Sustainable Development Goals (UN 2015) cover topics such as climate action (goal 13), clean water and sanitation (goal 6), life on land (goal 15), and good health and wellbeing (goal 3). An important future challenge will be to connect the environmental indicators developed and operationalised in the Life Cycle Initiative process, to these SDGs. In addition to exploring the application and utility of the indicators recommended in this report as a tool to support actions to improve the environmental situation and monitor the relative progress to selected sustainable development goals. Similarly, we strongly recommend exploring opportunities to make use of the environmental indicators for decision-making processes in the context of environmental planetary boundaries and in monitoring the environmental impacts of nations like the recently published report on environmental footprints of Switzerland and their development from 1996 to 2015 (Frischknecht et al. 2018).

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Glossary

Accessibility	Mass quantity of a chemical substance that is or can become available (e.g., for uptake by biota) within a given time span and under given conditions (Reichenberg and Mayer, 2006). For metals in porous media, it represents metal that is potentially able to cause ecotoxicity, that is, metal that can partition to solution
Adaptive capacity	The ability of individual species or an entire ecosystem to cope with environmental pressure and ability to maintain its structure and functions under changed environmental conditions during the exposure. It is mainly influenced by evolutionary changes (e.g., reproduction for genetic change) and plastic ecological responses (e.g., dispersal or behavioural changes), which are dependent on species or ecosystem specific factors, and duration or magnitude of the exposure (Williams et al. 2008; Nicotra et al. 2015; Beever *et al.* 2016)
Aggregated spatial scale	A transformation of the native spatial resolution to a new spatial resolution, usually at the country, continental, or global scale (Mutel et al. 2018)
Anthropogenic stock(s)	Stock(s) of resources within the technosphere
Background system	The background system consists of processes on which no, or at best, indirect influence may be exercised by the decision maker for which an LCA is carried out Such processes are called "background processes" (Clift et al. 1998)
Benchmark dose (BMD)	An estimate of a dose causing a specified level of response as estimated from a dose-response function fitted to a set of data on responses varying with different tested doses, adjusted by "uncertainty factors" to apply to a human population
Bioavailability	Mass quantity of a chemical substance that is freely available to cross an organism's cellular membrane from the medium the organism inhabits at a given time (Semple et al. 2004)
Biodiversity	Variability among living organisms from all sources including, inter alia, terrestrial, marine and other aquatic systems, and the ecological complexes of which they are part, including diversity within species, between species, and of ecosystems. (Article 2 of the Convention on Biological Diversity, UN 1992)
Biome	The world's major communities, classified according to the predominant vegetation and characterized by adaptations of organisms to that particular environment; for instance, tropical rainforest, grassland, tundra (Campbell 1996)
Biotic ligand model (BLM)	Ecotoxicity models for metals, which assumes that the ecotoxic response is proportional to the amount of metal ions bound to biotic ligand as influenced by dissolved protons and base cations in the water phase

Characterisation factor (CF)	Characterisation factor (CF) relates or translates the elementary flow into its impact on the chosen indicator for the impact category CFs are also referred to as comparative toxicity potentials (CTP) for those impacts that are related to chemical pollution
Concentration-response function (CRF)	The slope and/or shape of the relation between the frequency (rarely severity) of a selected health outcome in the target population versus (usually centrally) monitored concentration of a selected air contaminant
Conditions for maintained biodiversity (CMB)	These relate to key factors important for biodiversity, such as dead wood in a boreal forest (Michelsen 2008)
Continuous endpoint	A factor affected by a chemical exposure measured as a quantitative change in a measured feature (such as organ weight) – variable response
Cultural services	Benefits humans obtain from ecosystems that are non-material (e.g., recreation, aesthetic values, sense of place)
Depletion	In very general terms, "depletion" can be defined as, a reduction in the number or quantity of something. We use "depletion" with reference to stocks, whereas only a finite stock such as an ore body can be depleted
Dichotomous endpoint (stochastic and deterministic)	A factor affected by a chemical exposure measured as the rate of presence or absence of a defined effect (such as cancer) – yes/no response Deterministic dichotomous endpoint: Response is proportional to chemical exposure dose (e.g., alcohol intoxication) Stochastic dichotomous endpoint: Probability of response is proportional to chemical exposure dose (e.g., cancer)
Dissipation	Economically and technically irrecoverable loss of resources This definition is of current debate and dissipation is hard to quantify as the threshold for irrecoverability depends on future technologies and costs
Dose-response function (DRF)	Description of the relationship between the magnitude of a stressor (e.g., chemical exposure dose) and the response in a receptor population (e.g., humans) to show a certain effect (e.g., cancer)
EC10 equivalent (EC10eq)	Equivalent of chronic effect concentration affecting 10% of individuals above background The chronic EC10 equivalent comprehends the chronic endpoints NOEC, LOEC, MATC, EC50, and chronic ECx where x is between 1 and 20, adjusted by appropriate correction factors
Ecological vulnerability	Extent to which an ecosystem, at different levels of organisation (e.g., species, communities, ecosystems), may potentially experience alterations, expressed as potential impacts, resulting from an exposure to environmental stress
Economic reserves / mineral reserves	"The economic reserve is that part of the reserve base that can be economically extracted at the time of determination" (Guinée and Heijungs 1995)
Ecosystem	A dynamic complex of plant, animal and micro-organism communities and their non-living environment interacting as a functional unit (Article 2 of the CBD, UN 1992)

Ecosystem services	The benefits people obtain from ecosystems. These include provisioning services such as food and water; regulating services such as flood and disease control; cultural services such as spiritual and recreational benefits; and supporting services such as nutrient cycling that maintain the conditions for life on Earth (MEA 2005, p. 895)
Effect dose inducing a 10% response over background (ED10)	An estimate of the dose causing a 10% response (a response rate for dichotomous endpoints, a fractional change for continuous endpoints) based on a dose-response function fitted to data on responses at different tested doses
Effect dose inducing a 10% response over background for the human population ($ED10_H$)	An ED10 that has been adjusted to apply to a human population
Endemic species	See Endemism
Endemism	Association of a biological taxon with a unique and well-defined geographic area (The Encyclopedia of Earth 2016)
Exergy	"The exergy of a system or resource is the maximum amount of useful work that can be obtained from this system or resource when it is brought to equilibrium with the surroundings through reversible processes in which the system is allowed to interact only with the environment" (Dewulf et al. 2008)
Far-field environment	Environment that is distant from workers or consumers including environmental media (e.g., ambient air, freshwater, and soil), biota (e.g., agricultural crops, wild animals, and plants), or technological systems (e.g., waste water treatment plants and landfills) (Fantke et al. 2016)
Final ecosystem services	Refer to the point in which a service is enjoyed or benefited by humans, or to the last measured contribution of the ecosystem to human well-being or ecosystem quality
Foreground system	The foreground system consists of processes that are under the control of the decision maker for which an LCA is carried out. These processes are called "foreground processes" (Clift et al. 1998)
Free ion activity model (FIAM)	Ecotoxicity model for metals, which assumes that the ecotoxic response is proportional to metal free ion activity in the water phase
Functional diversity	Set of functions that organisms perform in a specific level of organisation, such as an ecosystem
Global burden of disease (GBD)	Study series that comprehensively assesses regional and global human mortality and disability from major diseases, injuries, and risk factors
Habitat	The place or type of site where an organism or population naturally occurs (Article 2 of the CBD Convention on Biological Diversity, UN 1992)
Hotspot, hotspot analysis, LCA	Within an LCA study, a hotspot is a relevant environmental aspect and its position in the life cycle A hotspot analysis covers the identification of relevant processes and potential impacts for further investigation within the LCA study
Instrumental values	The values that represent means for human purposes
Intake fraction (iF)	The proportion of an agent that is emitted or released into the environment, which is eventually inhaled, ingested or dermally absorbed by the human population (Bennett et al. 2002)

Intermediate products	"Product, material, or energy flows occurring between unit processes of the product system being studied" (ISO 2006)
Intrinsic values	The values assigned to the existence of an entity in itself, i.e., the values inherent to nature independent of human judgement. Intrinsic values therefore imply that entities have a value simply for what they are
LANCA®	Land use impact method developed by Fraunhofer-Institut für Bauphysik
Life Cycle Assessment (LCA)	Compilation and evaluation of the inputs, outputs, and the potential environmental impacts of a product system throughout its life cycle (ISO 2006)
Mineral resources	Chemical elements (e.g., copper) or minerals (e.g., gypsum) or aggregates (e.g., sand) as embedded in a natural or anthropogenic stock
Natural resources	"Material and non-material assets occurring in nature that are at some point in time deemed useful for humans" (Sonderegger et al. 2017)
Near-field environment	Indoor or near-consumer environment within the vicinity of the use of a considered product ('user' environment) including indoor air, consumer products and objects, and their surfaces (Fantke et al. 2016)
New approach methodologies (NAM)	A set of techniques to estimate effects of chemical exposure on human health; originally used to replace methods based on animal testing
$PM_{2.5}$	Fine particulate matter referring to particles with aerodynamic diameter ≤2.5 μm
Point of departure (POD)	Point on a toxicological dose-response curve established from experimental data or observational data generally corresponding to an estimated effect response level.
Primary or natural mineral resources	Chemical elements (e.g., copper) or minerals (e.g., gypsum) or aggregates (e.g., sand) as embedded in natural stocks, e.g., copper in an ore
Primary raw material	Material extracted from primary or natural mineral resources, e.g., copper ore
Product intake fraction (PiF)	Chemical mass within a product that is eventually taken in by humans per unit of chemical mass in that product (Jolliet et al. 2015)
Provisioning services	The products obtained directly or indirectly from ecosystems (e.g., food, fibre, genetic resources) (MEA, 2005, p. 897)
Quantitative structure-activity relationship (QSAR)	One of various mathematical models that estimate the ability to cause toxic effects or potency based on the chemical's molecular structure
Raw material	Material extracted from mineral resources
Reactivity (of a metal)	Ability of a metal in the solid phase to equilibrate with the solution phase within a few days (Degryse et al. 2009). The reactive metal typically includes outer-sphere and weakly bound inner-sphere complexes on mineral surfaces or organic matter and should not be confused with the "chemically labile" metal. The latter may include strongly sorbed inner-sphere complexes, which are chemically reactive, but not necessarily available for solid-liquid partitioning within a time scale of days
Recovery potential	Time needed and the extent to which an ecosystem or individual species can reach a new equilibrium state after the exposure (e.g., reproduction for repopulation). It is dependent on species or ecosystem specific factors, the ecosystem quality state of the surrounding system, and the ecosystem quality state after the exposure (van Nes et al. 2007)

Reference state	Reference state is a baseline used as a starting point to which to quantitatively compare another situation. A reference state can be, for example, a (hypothetical) situation representing conditions in the absence of human intervention, an anticipated or desirable target situation, or the current situation. A reference state refers to a time period and space
Regulating services	The benefits obtained, directly or indirectly, from the regulation of different ecosystem processes (e.g., climate regulation, erosion regulation) (MEA, 2005, p. 897)
Secondary or anthropogenic mineral resources	Chemical elements (e.g., copper) or minerals (e.g., gypsum) or aggregates (e.g., sand) as embedded in anthropogenic stocks (e.g., copper) in electronic waste
Secondary raw material	Material extracted from secondary or anthropogenic mineral resources, e.g., copper scrap
Sensitivity	Degree to which an ecosystem or individual species is affected by the exposure to a pressure
Speciation	For metals, ability of a metal to exist in different chemical forms, as interconverting species that can vary in toxicity
Supporting services	Ecosystem services that are necessary for the production of other ecosystem services (e.g., biomass production, soil formation, nutrient cycling) (MEA, 2005, p. 898)
Taxonomic group	Group of related organisms, according to similar biological characteristics
Threat level (threatened status)	Indicator of the conservation status of species, according to a set of defined criteria, which evaluate the extinction risk of species (IUCN 2001)
Threshold of toxicological concern (TTC)	Principle that refers to the establishment of a generic exposure level for all chemicals below which there would be no appreciable risk to human health (Kroes et al. 2005)
Ultimate reserves / crustal content	Total stocks of resources in the earth's crust (Guinée and Heijungs 1995)
Ultimately extractable reserves / extractable global resource	Fraction of ultimate reserves that can be technically extracted "However, data on this type of reserve are unavailable and will never be exactly known because of their dependence on future technological developments" (Guinée and Heijungs 1995)
Vulnerability	1) Vulnerability is the degree to which a system is susceptible to, and unable to cope with, adverse effects of environmental damages. Vulnerability is a function of the character, magnitude, and rate of environmental damage and variation to which a system is exposed, its sensitivity, and its adaptive capacity (adapted from http://climate-adapt.eea.europa.eu/glossary#linkVulnerability, data accessed 18/03/2016) 2) The propensity or predisposition to be adversely affected. Vulnerability encompasses a variety of concepts including sensitivity or susceptibility to harm and lack of capacity to cope and adapt (IPCC 2014, p. 128) 3) Vulnerability is a broad term encompassing concepts such as rarity, resilience and recoverability of e.g., species or ecosystems

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Peer Review report

Prepared by Technical Review Committee Chair, Experience Nduagu, University of Calgary, Canada, 31st May 2019, New Jersey, USA

An ad hoc Technical Review Team (TRT) was appointed by the Steering Committee of the Global Guidance for Life Cycle Impact Assessment, Volume 2 (a collaboration of the Life Cycle Initiative and SETAC). The ad hoc TRT was charged with the responsibility of meeting quality standards and ensuring that the review process is robust, followed international acceptable standards and is consistent with the deliverables on life cycle methodologies and on issues of scientific and policy concern. The TRT ensures that the final report is consistent with the missions and objectives of the Pellston Workshop on Life Cycle Impact Assessment which took place in Valencia, Spain on 24-29 June 2018.

This section presents a quality report prepared by Experience Nduagu (University of Calgary, Canada), TRT Chair for the Global Guidance on Environmental Life Cycle Impact Assessment Indicators – Volume 2. The peer review report is a summary and assessment of the review process and outcomes.

Background

This report is the Volume 2 of the Guidance for Life Cycle Impact Assessment which is a follow up of the Part I report on "Pellston Workshop Environmental LCIA Indicators", published in 2016. The SETAC Pellston Workshop on the LCIA Indicators, Volume 1, was followed by a preparatory stage of work for the Pellston Workshop on Global Guidance for LCIA Indicators, Volume 2. These preparatory assignments, which were led by individual task forces for the five impact category areas include topical stakeholder meetings, workshops, and conferences that scoped and developed the environmental indicators. The outcomes of the activities of each task force were documented in white papers that formed the background document for the Pellston Workshop.

The SETAC Pellston Workshop marked the second stage of work. Its primary objective is to reach consensus on recommended environmental indicators and characterisation factors for Life Cycle Impact Assessment (LCIA) in the following areas: acidification and eutrophication; human toxicity; ecotoxicity; soil quality and related ecosystem services; mineral resources; and cross-cutting issues. The Pellston Workshop produced a draft report of consensus of experts and stakeholders on the recommended environmental indicators for each impact category.

The chair and members of the TRT did not directly participate in the Pellston Workshop but some substance reviewers had participated in previous stakeholder discussions; they are aware of the overall progress made. The Chair of TRT notes that in these processes, serious attention was given to finding a good balance between the perspectives of business, industry, academia and other stakeholders. The list of participants in the process reflects a balance of perspectives in terms of affiliation, geography, and gender.

The TRT acted as an independent advisory resource and reported back to the Steering Committee. The TRT consists of men and women from a diverse mix of domain experts and users' expertise.

Technical Review team

The TRT comprises of a minimum of two substance reviewers for each of the six topical tracks, and in some cases up to four reviewers who took part in the technical review. The following are the TRT mandates: 1) Verify the accuracy of the science and proposal in the report, 2) Ensure an alignment of the activity with the original project goals and objectives, 3) Highlight unclear points that need scientific and editorial modifications, 4) Follow ISO-style review template in presenting their comments and concerns, and 5) Ensure an adequate balance of geographic representation and gender, as well as field of expertise in the review process.

In January 2019, Dr. Experience Nduagu, University of Calgary, was asked to act as the TRT Chair of the Life Cycle Initiative's Global Guidance on LCIA indicators. Between January and February 2019 substance reviewers were also appointed by the Steering

Committee. The substance reviewers were given 3 weeks to complete their tasks and submit their comments to the TRT Chair who then compiles and relays the received comments to the authors. The entire technical review process took place between March and June 2019. The contribution of the TRT members is recognized in the acknowledgment section of this report.

Peer Review of the Draft Report

The technical review of the draft report followed a standard peer review approach where the chapters of the draft report (from the Pellston Workshop) and a review template were sent to the substance reviewers. The reviewers returned their comments in an ISO-style review template where the following are tabulated: 1) reviewers' comments and justification for change, 2) proposed change by the reviewer and 3) author`s observations on each of the reviewer's comments.

The reviewers were advised to focus on the intent of the review, which is to verify the accuracy of the science, findings, and recommendations in the report and assure a high level of quality and international recognition of the work. The reviewers were further asked to avoid suggesting major rewrites and editorial-focused modifications. However, in many cases, editorial modifications were made by the reviewers using track changes and mark-ups in the report. A once-through review process sufficed for all but one of the chapters were major science-based changes were suggested which led to a second review.

The comments received from the reviewers were addressed satisfactorily by the authors of the chapters. The modified chapters together with the completed ISO-styled summary review template were returned the TRT Chair who determined whether the authors satisfactorily addressed the comments. When this condition is met, the finalized chapters and the accompanying review comments are compiled by the TRT Chair and forwarded to the UNEP/SETAC office for editorial review and final publication process.

TRT Chair Recommendation

The peer review process was generally positive and constructive, resulting in both scientific and editorial improvements of the report while maintaining the substance and spirit agreed by the workshop in Valencia. A majority of the comments focused on improving the clarity of some scientific statements and synching segments of the chapters and the entire report.

The reviewers were intentioned in their efforts to verify the accuracy of the science and proposal and to highlight unclear points that need modifications. In many instances, the reviewers demanded that the authors provide scientific basis and references to support certain assertions or update dated references.

Since the report emanated from a process that requires some level of consensus, which means that an absolute consensus among experts was not necessary, the review process ensured that the concepts, principles, and recommendations are supportable and defensible. It must be noted that some of the indicators and frameworks still require further scientific and practical validation. For this reason, the workshop process rules stipulate different levels of recommendations based on the maturity of the methods and applicability.

It is commendable that the report highlights where disagreements exist, documenting different and minority opinions. In some instances, the reviewers challenged the recommendations in the report and provided reasons for their disagreements and in other cases, reviewers suggested additional recommendations. In these cases, the authors provided an explanation in support of the adopted recommendation and why new recommendations cannot be made at this point. New recommendations or major changes to the content of the report were avoided following the Pellston process which provides no option for a major rewrite of the text. Detailed comments and responses to the individual comments can be obtained from the Secretariat of the Life Cycle Initiative.

Review statement

In general, the Pellston Workshop process was followed and the final revised document produced from this process fulfils the set objectives. The process facilitated a rich collaboration of experts from academia, industry, government and other organizations which resulted in expanding scientific discussion and knowledge, culminating in the global guidance for LCIA, Volume 2. The TRT fully expects that this report will be valuable in further advancing the science and application of life cycle modelling in the five topical areas addressed.

Note from the editors:

All peer review comments were assessed and incorporated when deemed appropriate and relevant. The complete set of comments submitted by the peer reviewers are available upon request from info@lifecycleinitiative.org.

List of Public Stakeholder Consultation Events

International Symposium on Life Cycle Impact Assessment: Towards development of global scale LCIA method

Yokohama, Japan | 23 November 2012

Open stakeholder consultations: Global guidance on environmental life cycle impact assessment indicators

Glasgow, United Kingdom | 16–17 May 2013

Basel, Switzerland | 15 May 2014

Barcelona, Catalonia, Spain | 7 May 2015

Special session of the SETAC Europe 26th Annual Meeting: Consensus building in life cycle impact assessment

Nantes, France | 25 May 2016

Life Cycle Impact Assessment Workshop at V Brazilian Life Cycle Management Congress

Fortaleza, Brazil | 19 September 2016

Special session of the V Brazilian Life Cycle Management Congress: UNEP/SETAC Consensus Methods for LCIA

Fortaleza, Brazil | 21 September 2016

Special session of the LCA XVI conference: The UNEP/SETAC Life Cycle Initiative flagship project on Global guidance on environmental life cycle impact assessment indicators

Charleston, SC, USA | 27 September 2016

Special session of the Eco-balance conference: The UNEP SETAC Life Cycle Initiative flagship project on Global guidance on environmental life cycle impact assessment indicators

Kyoto, Japan | 6 October 2016

Open stakeholder consultations: Global guidance on environmental life cycle impact assessment indicators

Brussels, Belgium | 11 May 2017

Rome, Italy | 16 May 2018

Presentation (Cecile Bessou) and feedback at the ILCAN Workshop IC SOLCA: Consensus building on LCIA 2nd Pellston Workshop

Jakarta, Indonesia | 24–25 October 2018

Open stakeholder consultation at the SETAC North America 39th Annual Meeting: Global Guidance on Environmental Life Cycle Impact Assessment Indicators 2nd consensus building on LCIA Sacramento, California, USA | 7 November 2018

About the Life Cycle Initiative

The Life Cycle Initiative is a public-private, multi-stakeholder partnership enabling the global use of credible life cycle knowledge by private and public decision makers.

Hosted by UN Environment, the Life Cycle Initiative is at the interface between users and experts of life cycle approaches. It provides a global forum to ensure a science-based, consensus-building process to support decisions and policies towards the shared vision of sustainability as a public good. It delivers authoritative opinion on sound tools and approaches by engaging its multi-stakeholder partnership (including governments, businesses, scientific and civil society organizations, and individuals).

The Initiative facilitates the application of life cycle knowledge in the global sustainable development agenda to achieve global goals faster and more efficiently.

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