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Life Cycle & Sustainability

Assessment of the sustainable use of chemicals on a level playing field

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Abstract

Misleading conclusions can result from applying tools beyond the purposes for which they were designed. A range of chemical assessment systems was compared against a set of principles germane to the sustainable use of chemicals relevant to the whole societal life cycles of finished products. These principles of sustainable use included: wider dimensions of sustainability, a foundation in science, consideration of life-cycle risk rather than simply intrinsic chemical properties, contributions to meeting human needs, open access, and peer review. A transparent basis in science is important for deriving objective, comparable, and replicable sustainability-based findings across materials and applications, and for guiding innovation. Few assessment systems currently identify how use of substances contributes to meeting human needs, a vital albeit often overlooked aspect of sustainable development, with most based largely on potential hazard without addressing wider life-cycle exposure and risk assessment. Qualitatively differing substances were illustratively assessed against the sustainability principles and life-cycle context of the Additive Sustainability Footprint (ASF), aspects of this analysis highlighting how differing material sourcing, manufacturing, and management in-use and at end-of-life can lead to widely divergent sustainability assessments. These illustrative ASF assessments also demonstrate that material use challenges, assessed on a systemic basis, are common across materials, with no defensible automatic assumption that there are inherently "good" or "bad" materials; differing stewardship across whole product life cycles substantially influences sustainability credentials for all materials. It is therefore important that the sustainability performance of all materials is assessed on an objective "level playing field," which also highlights "hot spots" for sustainable innovation from supply-chain management through manufacturing, substance selection by material compounders, maintenance inputs in product use, and beyond product end-of-life. Chemical regulation must evolve to include and embed wider sustainability principles into operational practice and become applicable and enforced across increasingly global value chains. *Integr Environ Assess Manag* 2023;19:1131–1146. © 2022 The Authors. *Integrated Environmental Assessment and Management* published by Wiley Periodicals LLC on behalf of Society of Environmental Toxicology & Chemistry (SETAC).

KEYWORDS: Additives; Additive Sustainability Footprint (ASF); legislation; life-cycle assessment; sustainable development; The Natural Step

INTRODUCTION

Assessment systems and their associated metrics are developed to serve specific purposes. Misapplication or incautious transfer of findings from any assessment system to a purpose for which it is not designed can generate misleading outcomes based on wrong assumptions. These principles are relevant to assessment systems and approaches used in the chemicals sector.

Disclosure of chemical ingredients and their related toxicological hazard characteristics is increasingly prevalent in consumer products (Target, 2013; Walmart, 2014). Panko et al. (2017) applied a range of commonly applied assessment tools to seven chemical substances selected to represent both natural and synthetic chemistries and with differing toxicological activity, finding that the selected tools differed widely in their classifications of the same chemical substances. Although assumed to represent "greenness," Panko et al. (2017) highlight how these tools differ in the sources of information used to judge hazard in isolation, application of hazard characteristics of single chemical ingredients to whole consumer products, consideration of the chemical's functional role, or potential for human exposure. Only one of these tools, SciVera Lens, was found capable of providing estimates of chemical exposure and risk

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characterization using a hazard quotient approach. However, this characterization was only an optional element of SciVera and was applied solely to chemicals already ranking as of very high or high hazard in CMR (carcinogenic, mutagenic, reprotoxic) categories.

The importance of accounting for sustainability across full product life cycles is increasingly acknowledged, for example by the German Federal Environment Agency (2009). Distinguishing risk, accounting of exposure in the life cycle, from potential hazard alone is important for determining the safety of chemicals in practical use. Some substances may be fully consumed or contained in manufacturing, bound into products, and/or recovered by recycling at end-of-life, eliminating or limiting exposure and thus risk across product life cycles. Shifting emphasis from intrinsic properties to use-related risk across full societal life cycles of the products into which chemicals are embedded is therefore highly germane to choices and innovations contributing practically and transparently to progress with sustainable development. This includes post-use phases including potential for recycling and the existence of infrastructure to achieve it practically. Assessments based on intrinsic chemical properties outside the wider context of use cannot be safely assumed to represent sustainability, although they can help identify and prioritize the removal of the most seriously damaging substances. However, many substances with a lower potential for hazard that are commonly used to support society's needs may pose low risks when exposure is assessed in the context of the full life cycles of products into which they are integrated and the availability of societal infrastructure for their management. A logical objective for sustainable development is an assessment approach that addresses the potential roles that chemicals can play in supporting human needs in the safest and most materially efficient ways. Risk-based selection decisions are therefore necessarily context specific, considering wider factors such as containment in manufacturing processes, complete consumption or conversion during manufacturing or compounding, and immobilization in compound matrixes allowing recovery through recycling or safe disposal without release. Some chemical assessment approaches are based substantially on hazard criteria, limiting their value for wider sustainability assessment. Some others described as taking a risk-based approach are initially founded on assessment of the intrinsic properties of substances, with socioeconomic considerations introduced later in implementation (e.g., see Annex A).

Some materials in common societal use, including for example polyvinyl chloride (PVC) and its additives, addressed in a case study later in this article, have been subjected to a disproportionately high level of scrutiny. This can lead to often-unfounded perceptions that these materials are qualitatively distinct from others used by society, and with an entirely unique set of sustainability challenges. However, a rapid assessment of the performance of selected alternative materials used in widespread PVC applications—timber and/or forest-based products (window profiles), ductile iron (water pipes), and polyolefins (pipes and cables)—using a set of five linked, science-based sustainability challenges identified that these challenges were common to all assessed materials (Everard, 2020). (The five linked sustainability challenges published by Everard et al. [2000] include: carbon neutrality, controlled-loop system, releases of persistent organic compounds across product life cycle, use of additives including maintenance inputs across product life cycles, and awareness of sustainable development across the whole value chain). The durability, longevity, and low requirement for maintenance inputs during PVC product life and potential recyclability in some cases was concluded to offer significant sustainability advantages over alternatives (Everard, 2020). A further consequence of the disproportionately high scrutiny of some materials is that alternative materials may tend to receive a lower degree of scrutiny, regulation, and voluntary control with respect to sustainability criteria and can wrongly be assumed to be more sustainable.

In order to make practical and transparently corroborated progress with sustainable development, it is necessary to address all materials and their constituents on a level playing field of common criteria relevant to sustainable choices and innovation, relevant across geopolitical regions. A basis of common, sustainability-relevant assessment criteria can overcome oversimplistic decision-making based on perceptions often promoted by media and nongovernmental organizations (NGOs), and publicity that is not founded on clear and defensible principles. This article seeks to identify the characteristics of assessment systems robustly informing the sustainable use of chemical substances across whole product life cycles. It achieves this by comparing assessment systems commonly used to address aspects of chemical safety and sustainability against a set of principles relevant to assessment of sustainability risk across whole product life cycles. These principles include both potential negative consequences but also positive contributions of the use of these substances to addressing human needs. A range of materials with differing properties is then compared illustratively against one assessment system found to embody all sustainability-relevant criteria highlighting insights that can be derived from a systemic approach to the use of chemical substances.

METHODS

Selection of chemical assessment systems and sustainable development criteria

A range of established assessment systems and approaches used commonly in the chemicals sector was identified for testing against a set of criteria relevant to sustainable development. These are listed, with a summary of their purposes, in Table 1. Criteria considered important for overall sustainable development assessment are listed in Table 2, together with a rationale for their inclusion.

Authoritative sources for these assessment schemes are listed in Table 1, and these were reviewed for the extent to which the criteria relevant to sustainable development in Table 2 were addressed. These were assigned as being met

TABLE 1 Selected assessment systems used in the chemicals sector with their purposes

Tool and/or approach	Purpose
Life-cycle assessment (LCA)	LCA, as characterized by ISO 14040:2006 (ISO, 2006), describes the principles and framework for life-cycle assessment including: definition of the goal and scope of the LCA, the life-cycle inventory analysis phase, the life-cycle impact assessment phase (mainly in practice related to toxicological and negative environmental implications), the life-cycle interpretation phase, reporting and critical review of the LCA.
Environmental product declaration (EPD)	An EPD is a standardized document containing information about a product's potential environmental and human health impact, based on LCA calculations providing a quantitative basis for comparison of products and services. Environmental product declarations must be verified by an independent expert, normally with a validity of five years. Environmental product declarations are “Type III environmental declarations” under ISO 14025:2006 (ISO, 2020).
Product environmental footprint (PEF)	PEF is a multicriteria measure of the environmental performance of a good or service throughout its life cycle, presenting a common framework to assess extraction of raw materials, production, use, and final waste management and including flows of material and/or energy and the emissions and waste streams associated with a product throughout its life cycle (EC, 2012).
EU REACH	EU REACH regulations (EC, 2008) aim to improve the protection of human health and the environment through the better and earlier identification of the intrinsic properties of chemical substances through the four processes forming the acronym: Registration, Evaluation, Authorisation, and restriction of CHemicals. REACH also aims to enhance innovation and competitiveness of the EU chemicals industry (EC, 2006). Manufacturers and importers are required to gather information on the properties of their chemical substances and to register the information in a central database held by the European Chemicals Agency (ECHA). European Commission (n.d.) describes how “better and earlier identification of the intrinsic properties of chemical substances” (hazard-based assessment without consideration of exposure) operates through its four constituent processes of Registration, Evaluation, Authorisation, and Restriction, with risk-based and economic considerations only applied at the end of this flow once intrinsic properties have led to recommendation for substitution.
SciveraLENS	SciveraLENS is operated by a commercial company (SciveraLENS, 2022) screening chemical formulations using 23 toxicological endpoints to identify potential issues, with the intent of finding safer alternatives and simplifying compliance and certification requirements. Essentially, this is a list-based approach founded on potential hazards.
GreenSuite	GreenSuite is a patented, web-based application claiming to deliver an integrated environmental solution customized to specific business needs addressing environmental issues at all points of supply chains from premanufacture notifications and Material Safety Data Sheet generation, to emissions monitoring and waste disposal, taking account of global regulatory change (GreenSuite, 2022).
GreenScreen List Translator	GreenScreen List Translator is a list-based hazard screening approach, essentially representing a “list of lists” approach to quickly identify chemicals of high concern, scoring chemicals based on information from more than 40 hazard lists developed by other bodies (including governmental agencies, intergovernmental agencies, and nongovernmental organizations (NGOs) (GreenScreen, 2022). GreenScreen Assessment is a chargeable service.
GreenWERKS	GreenWERKS is a software screening tool commercially available for chemical manufacturers, originally introduced in conjunction with Walmart in May 2009, for evaluating consumer products. Originally based on a 2009 USEPA list of “chemicals of concern,” this approach is essentially another “list of lists” screening applications. The GreenWERKS approach is based on a user-defined configuration allowing organizations to set their own criteria for greener chemistry (Environmental Expert, 2010).
Green Chemistry and Commerce Council (GC3) Retailer Database	The GC3 Retailer Database includes a range of variously free or commercially available tools intended to help retailers select safer or “greener” products based on lists of substances with potential human health and environmental

(*Continued*)

TABLE 1 (*Continued*)

Tool and/or approach	Purpose
	impacts, including both regulated substances and others of concern though not yet regulated (Green Chemistry and Commerce Council [GC3], 2022).
OECD Substitution and Alternatives Assessment Toolbox (SAAT)	The OECD Substitution and Alternatives Assessment Toolbox (SAAT) is a compilation of resources relevant to chemical substitution and alternative assessments, divided into four "resource areas" (Organization of Economic Co-operation and Development [OECD], 2022). These are: Alternatives Assessment Tool Selector (filterable inventory of chemical hazard assessment tools and data sources); Alternatives Assessment Frameworks (summary of the current frameworks that can be used to assess alternatives); Case Studies and Other Resources; and Regulations and Restrictions (listing regulations and restrictions throughout OECD member countries). Essentially, this is a "list of lists" and a "framework of frameworks" relating to chemical hazard and restrictions.
ECHA plastic additives initiative	The ECHA plastic additives initiative (European Chemicals Agency [ECHA], 2018) extends focus across all polymers, making up a report characterizing the uses of plastic additives and the extent to which 400 additives used in plastics at high volumes in the EU may be released from plastic articles. This method helps companies determine which registration dossiers they should update as highest priority and to identify where safe-use information communicated down the supply chain must be further improved. Practical Guide is available for registrants.
Cradle to Cradle	Cradle to Cradle is a commercial tool aiming to influence design of products relating to their safe, circular, and responsible manufacture across the five criteria: material health (safe for humans and the environment), product circularity, clean air and climate protection, water and soil stewardship, and social fairness (Cradle to Cradle Products Innovation Institute, 2022).
Additive Sustainability Footprint (ASF)	Developed for assessment of the sustainability of the use of PVC additives across whole PVC article life cycles and founded on scientific sustainability principles applied at each life-cycle stage, ASF is built on preexisting tools with generic applicability to chemicals (Everard & Blume, 2019).
Ecovadis	Ecovadis is a commercial service providing holistic sustainability ratings of companies covering a broad range of nonfinancial management systems including environmental, labor and human rights, ethics, and sustainable procurement impacts (Ecovadis, 2022). Evidence-based assessments are via scorecards (0–100 scores) and medals (bronze, silver, gold) when applicable, that may be used as an outsourced sustainability platform to improve sustainability performance, including influencing supply chains to go beyond compliance.
Carbon Handprint	Carbon Handprint assessment is used to calculate the greenhouse gas impacts of a product when used by a customer, essentially helping them reduce their carbon footprint, achieved by comparing the carbon footprint of the baseline solution with that of the carbon handprint solution when used by a customer (Pajula et al., 2018).
Material flow cost accounting (MFCA)	Material flow cost accounting (MFCA), defined in ISO 14051:2011, provides a general framework accounting for the flows and stocks of physical units of materials within an organization and the costs associated with those material flows, potentially extended upstream and downstream in value chains, and potentially generating financial benefits and reducing adverse environmental impacts from material throughput (ISO, 2011).
GRI 301: Materials	The "GRI 301: Materials" standard is part of the set of GRI Sustainability Reporting Standards (GRI Standards) designed to be used by organizations to report their impacts on the economy, the environment, and society. GRI 301 addresses the topic of materials including inputs used to manufacture and package an organization's products and services, accounting for nonrenewable and renewable material use, and the organization's approach to recycling, reusing, and reclaiming materials, products, and packaging (Global Sustainability Standards Board [GSSB], 2016).

TABLE 2 Criteria relevant to sustainable development assessment with rationale

Criterion	Rationale
Full dimensions of sustainable development	Social, economic, and environmental criteria are relevant to sustainable development, rather than any narrower aspect (such as toxicity) addressed in isolation
Transparently science-based	A robust basis in science is essential to avoid subjectivity or opinion
Hazard and/or life-cycle risk	Risk across whole article life cycles accounts of exposure, which may mean that potentially hazardous substances do not pose threats because of low or no exposure
Positive contributions to the meeting of human needs	In additional to negative implications, chemical substances are used to promote beneficial outcomes with positive sustainability benefits
Open access	If the methods are not openly communicated, replicability and testing cannot be achieved
Free to use (albeit with potential commercial guidance and external auditing)	The broad principles need to be testable (even if disciplined application of the tool and/or approach may require investment in training and auditing)
Applicable across products and/or materials	To be useful across applications, the tools and/or approaches need to be flexible for use across products and materials
Peer-reviewed	Peer-review in external scientific literature is a gold standard for testing scientific credibility. This assessment was undertaken through a structured search using the tool name, carried out on all leading science and legal databases linked from the University of the West of England library resources (May 2022). No comment is passed here as to whether the literature assesses the method as authoritative or flawed

(YES), partially met (Partially), or not met (NO), emphasized by color coding in Table 3 in the Results section, with explanatory details in Supporting Information: #01.

Application of ASF to illustrative case studies

The analysis of chemical assessment systems compared with sustainable development criteria (see Results section) found that Additive Sustainability Footprint (ASF) addressed all selected sustainable development criteria. This is because ASF took a full life-cycle approach, evaluating both negative and positive contributions of the use of chemical substances against wider dimensions of sustainable development (aspects of pollution, depletion, and ethics as covered by the four System Conditions of The Natural Step [TNS]) in the context of the whole societal life cycles of the products into which they are incorporated. (The TNS System Conditions: in a sustainable society, nature is not subject to systematically increasing: SC1: concentrations of substances extracted from the earth's crust; SC2: concentrations of substances produced by society; SC3: degradation by physical means; and in that society SC4: there are no structural obstacles to people's health, influence, competence, impartiality, and meaning-making). See Supporting Information: #02 for an overview of the history, purpose, and further characteristics of ASF, and also the peer-reviewed paper by Everard and Blume (2019).

To develop a deeper understanding of how more systematic approaches to assessment of the sustainable use of chemicals can develop insights about both challenges and opportunities, and so serve as a level playing field for chemical assessment, principles underpinning ASF were applied on an illustrative basis to a range of substances selected for their widely differing chemistry and environmental and ethical issues. These selected substances were: polymer additives (both metal-based PVC stabilizers and brominated flame retardants in polyolefins), timber used in window profiles representative of a biologically based material, and cobalt used in solar panels but with known ethical and environmental issues in the supply chain. These substances were considered for both potential negative (impact) and positive (progress) implications, also observing opportunities for mitigation, from different parts of the life cycle from raw materials extraction to end-of-life recycling or disposal as stratified against the four TNS System Conditions (sustainability principles).

RESULTS

Testing of chemical assessment systems against principles relevant to sustainable development

Table 3 summarizes findings of the more detailed analysis in the Supporting Information spreadsheet when selected chemical assessment systems and/or approaches are assessed for their coverage of criteria relevant to sustainable use.

Only three assessment systems (Cradle to Cradle, ASF, and Carbon Handprint) were found principally to address risk across full article life cycles, in preference to simpler evaluations extrapolating from the intrinsic properties of constituent substances. Only three assessment systems (Cradle to Cradle, ASF, and Ecovadis) included full dimensions of sustainable development. Approximately half of the assessment systems reviewed have been subject to peer-review. Only EU REACH is statutory although, despite

TABLE 3 Summary of assessments of chemical assessment systems and/or approaches in terms of their coverage of criteria relevant to sustainable use, emphasized by color coding (WHITE: Yes, fully meets criterion; MID GRAY: Partially meets criterion; DARK GRAY: No, does not meet criterion)

	Full dimensions of sustainable development	Transparently science-based	Based on full article life cycle risk (rather than potential hazard alone)	Recognises positive contributions to meeting human needs	Open access	Free to use (albeit with guidance and external auditing)	Applicable across products/ materials	Statutory	Peer reviewed in science literature
Life Cycle Assessment (LCA)	NO	YES	Partially	NO	Partially	Partially	YES	NO	YES
Environmental Product Declaration (EPD)	NO	YES	Partially	NO	Partially	YES	YES	NO	YES
Product Environmental Footprint (PEF)	NO	YES	Partially	NO	Partially	YES	YES	NO	YES
EU REACH	NO	YES	NO	NO	YES	YES	YES	YES	YES
SciveraLENS®	NO	YES	Partially	NO	NO	NO	YES	NO	NO
Greensuite®	NO	YES	Partially	NO	NO	NO	YES	NO	YES
GreenScreen List Translator™	NO	YES	NO	NO	NO	NO	YES	NO	Partially
GreenWERKS	NO	YES	NO	NO	NO	NO	YES	NO	NO
Green Chemistry and Commerce Council (GC3) Retailer Database	NO	YES	NO	NO	Partially	Partially	YES	NO	NO
OECD Substitution and Alternatives Assessment Toolbox (SAAT)	NO	YES	NO	NO	Partially	Partially	YES	NO	NO
ECHA Plastic Additives Initiative	NO	YES	Partially	NO	YES	YES	Partially	NO	NO
Cradle to Cradle	YES	YES	YES	NO	NO	NO	YES	NO	YES
Additive Sustainability Footprint (ASF)	YES	YES	YES	YES	YES	YES	YES	NO	YES
Ecovadis	YES	YES	NO	NO	NO	NO	YES	NO	NO
Carbon Handprint	NO	YES	YES	NO	YES	YES	YES	NO	YES
Material flow cost accounting (MFCA)	NO	YES	Partially	NO	NO	NO	Partially	NO	YES
GRI 301: Materials	NO	YES	NO	NO	YES	YES	YES	NO	NO

references to risk, its four constituent Registration, Evaluation, Authorisation, and Restriction processes are substantially based on intrinsic properties of chemical substances (as discussed in the Introduction of this article), with wider socioeconomic facets of sustainability only applied after substances are scheduled for potential substitution, and without addressing the contribution of the use of substances to meeting human needs.

Only one assessment system (ASF) addressed the positive contributions of material use for meeting human needs, a crucially important yet generally overlooked consideration because the purpose of chemical use is to serve human needs and demands as framed, for example, by the UN Sustainable Development Goals (UN, 2022). This is particularly so for the roles of chemicals used in construction for addressing beneficial outcomes for SDG9 (industry, innovation, and infrastructure) and SDG11 (sustainable cities and communities), also contributing to wider SDGs such as SDG6 (clean water and sanitation) and SDG7 (affordable and clean energy).

Illustrative application of ASF to the use of a variety of chemical substances

Table 4 summarizes some of the range of sustainability issues potentially associated with the use of metal-based PVC stabilizer substances stratified by TNS System Condition set in the life-cycle context of ASF (derived from Everard, 2008; Everard & Blume, 2019). These issues include aspects of the life cycle wherein concerns ("impact question" issues) or benefits ("progress question" responses) arise as well as mitigation measures, either already in place or as further opportunity to drive greater progress toward sustainability. Table 4 illustrates some of the breadth of analysis of sustainability issues and opportunities related to substance use across whole product life cycles.

This ASF-based approach is applied on a comparative basis to the wider selected range of qualitatively differing materials subject to ASF assessment, highlighting an illustrative subset of life-cycle issues in Table 5. This is illustrative due to space limitations but also to avoid distraction from the primary purpose of this article of assessing how chemical assessment systems cover sustainability principles. However, it does reveal how a stratified ASF approach across all System Conditions (pollution, depletion, ethics) reveals how all materials have both challenges and benefits at different stages in product societal life cycles. Apparently eco-friendly materials such as timber have highlighted issues and potential mitigation measures associated with sourcing as well as potentially offering limited service life (net societal value delivery) with treatment inputs in use that may inhibit recycling. Meanwhile, substances often considered problematic may, in use, confer durability and longevity to products delivering a long service life and be amenable to value recovery through controlled-loop management at end-of-life. Intrinsic chemical properties are only part of the wider breadth of issues to be considered in wider-ranging sustainability assessment considering maximization of societal value in the safest and most eco-efficient manner across whole finished product life cycles.

DISCUSSION

The booming global human population (8 billion in November 2022 projected by UN, 2017, to rise to 9.8 billion by 2050), depending on a dwindling natural resource base (Brondizio et al., 2019; Millennium Ecosystem Assessment, 2005), means that substantive traction with sustainable development is an increasingly urgent priority. There is a pressing need for the meeting of human needs on a safer, more efficient basis per unit of material resource. Infighting between or prejudices about different types of material are unhelpful; the overriding need is to determine transparently what is the most sustainable option for material use in any specific product application across its full societal life cycle. To allow this transition, transparently science-based frameworks and systemic assessment systems are required to allow industry, regulators, and other institutions involved in material life cycles to frame selection and management decisions, and to steer innovation to progressively improve sustainability performance in fulfillment of human needs.

Sustainable development is served only by assessment systems founded on and transparently embodying a range of principles considering multiple dimensions of sustainable development and set in the context of risk associated with the use of substances across the whole societal life cycles of the products into which they are incorporated from supply chains and manufacturing to finished articles in use and beyond end-of-life.

Available chemical assessment systems differ in their framing characteristics

Many assessment systems have been developed to assess discrete aspects of the sustainability of chemicals. Most focus on environmental and toxicological aspects. Few address sustainable development on a systemic basis in terms of sustainable use as opposed to intrinsic chemistry, wider socioeconomic aspects, risk across the whole societal life cycles of the articles in which they are incorporated, and recognizing positive contributions to meeting human needs along with the potential for negative outcomes.

The analysis in this article reveals that many assessment systems focus only on discrete aspects of the wider picture of sustainable development. Assessment systems such as LCA, EPD, and PEF focus essentially on aspects of potential environmental and human toxicity related to the intrinsic properties of substances. Many assessment systems also do so only or predominantly in the context of potential hazard, for example, LCA, GreenScreen, and OECD SAAT, rather than risk that would require accounting for exposure throughout the societal life cycle of finished products from the outset of assessment. Distinguishing risk informed by use-related environmental and human exposure, rather than extrapolating potential hazard from intrinsic chemical characteristics, is important for sustainability appraisal both for chemical safety as well as to ensure that the benefits of using these substances are not dismissed. Consequently, misleading conclusions may be drawn if the findings from more narrowly framed hazard-based assessment systems are extrapolated uncritically to wider sustainable development contexts that they are not explicitly designed to address.

Sala et al. (2013) recognized the value of life-cycle thinking for sustainability assessment, discussing the state-of-the-art of an emerging life-cycle sustainability assessment

TABLE 4 Potential sustainability issues by TNS System Condition associated with the use of metal-based stabilizer additives in PVC, including potential positive (☺) and negative (☹) implications and mitigation measures (↑) at specific points in final PVC product life cycles

Life-cycle stages					
Raw materials acquisition	Additive production	Packaging and distribution	Compounding and/or converting	Product use and/or maintenance	Post-use management
TNS System Condition 1					
☹ Risk of persistent heavy metals released in mining	☹ Risk of metal release in manufacturing	☹ Risk of metal release in transport	☹ Risk of metal release in compounding	Risk not perceived as metals are immobile in PVC compound	☹ Risk of metal release in incautious disposal
☺ Cadmium or lead are both now phased out from manufacturing in Europe by voluntary commitment	↑ Controlled manufacturing with postindustrial waste recycling or safe disposal	↑ Tightly controlled transport	↑ Controlled compounding with postindustrial waste recycling or safe disposal		☺ Controlled-loop recycling means metals are contained for reuse
↑ Cease procurement from additive suppliers not signing up to European voluntary standards					
↑ Substitute with lights elements more abundant in nature, or derive from recycled metals					
TNS System Condition 2					
☹ Risks from exhaust fumes and oils during extraction	☹ Risks from exhausts or other emissions in manufacturing	☹ Emissions in transport	☹ Risks from emissions during compounding	☺ The resilience of stabilized PVC gives long service life with low maintenance, averting inputs during extended service life	☹ Risk of emissions in incautious disposal
↑ Use low-emission machinery that is well maintained	↑ Low-emission manufacturing with postindustrial waste recycling	↑ Tightly controlled transport to minimize risk	↑ Use low-emission machinery that is well maintained, with postindustrial waste recycled or safely disposed		☺ Controlled-loop recycling means emissions and material value are contained
TNS System Condition 3					
☹ Risks habitat loss and groundwater disturbance during extraction	☹ Habitat displacement by manufacturing operations, and risks to water systems	☹ Physical disruptions from transport	☹ Habitat displacement by compounding operations, and risks to water systems	☺ The resilience of stabilized PVC gives long service life with low maintenance, averting management activities and inputs damaging to nature (including reduced water use) during extended service life	☹ Risk of emissions in incautious disposal physically damaging ecosystems

(*Continued*)

TABLE 4 (*Continued*)

Life-cycle stages					
Raw materials acquisition	Additive production	Packaging and distribution	Compounding and/or converting	Product use and/or maintenance	Post-use management
↑ Ideally, switch to recycled metal sources avoiding physical impacts	↑ Seek water- and biodiversity-neutral design of plant and management systems	↑ Tightly controlled transport with full loads to minimize risks	↑ Seek water- and biodiversity-neutral design of plant and management systems		☺ Controlled-loop recycling means material value is contained and landfill is not required
↑ For virgin metals, switch to suppliers certified for best mining practice		↑ Select packaging that will not be landfilled	↑ Ensure that waste is diverted from landfill		
TNS System Condition 4					
☹ Potential health risks during extraction	☹ Potential health risks during manufacturing	☹ Potential health risks during transport	☹ Potential health risks during compounding	☺ The resilience of stabilized PVC gives long service life with low maintenance, supporting the meeting of diverse human needs during extended service life	☹ Health risks through incautious disposal
↑ Ensure that suppliers are audited for low-emission machinery and safe and ethical operating practices	↑ Ensure that manufacturing uses safe and well-maintained machinery with safe and ethical operating practices	↑ Ensure that transport uses safe and well-maintained machinery with safe and ethical operating practices	↑ Ensure that compounding uses safe and well-maintained machinery with safe and ethical operating practices		☹ Waste of material value through incautious disposal ☺ Controlled-loop recycling means material value are contained and safety is ensured ☺ Controlled-loop recycling also creates new employment opportunities

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TABLE 5 Illustrative examples of potential positive (☺) and negative (☹) sustainability implications and mitigation measures (🡅) at specific points in final product life cycles in the use of selected chemicals (with more complete summary of metal-based PVC additives for comparison)

Life-cycle stages					
Raw materials acquisition	Additive production	Packaging and distribution	Compounding/converting	Product use/maintenance	Post-use management
Use of metal-based stabilizer additives in PVC					
Risks of metal release (SC1), persistent emissions (SC2), physical damage (SC3), and associated health impacts (SC4) can be 🡅 contained by using recycled metal or best practice in virgin extraction	Risks of metal release (SC1), persistent emissions (SC2), physical damage (SC3), and associated health impacts (SC4) can be 🡅 contained by controlled manufacturing with postindustrial waste recycling	Risks of metal release (SC1), persistent emissions (SC2), physical damage (SC3), and associated health impacts (SC4) can be 🡅 contained by controlled efficient and tightly controlled transport	Risks of metal release (SC1), persistent emissions (SC2), physical damage (SC3), and associated health impacts (SC4) can be 🡅 contained by controlled compounding with postindustrial waste recycling or safe disposal	The resilience of stabilized PVC gives long service life with low maintenance, delivering societal value with low and/or no inputs	Risks of metal release (SC1), persistent emissions (SC2), physical damage (SC3), and associated health impacts (SC4) and resource wastage from incautious disposal can be 🡅 contained by controlled-loop recycling
Use of brominated flame retardants in polyolefins					
☹ Mining of chemicals used in manufacture of brominated retardants can disrupt landscapes and aquifers (SC3) though 🡅 bio-based manufacture potentially reduces this problem	☹ When based on mined petrochemicals, can lead to emission and accumulation of climate-active gases (SC2) though 🡅 bio-based manufacture potentially reduces this problem			☺ Flame retardants reduce fire-related human health risks	☹ Health risks (SC4) can occur if retardants are released during product disposal though 🡅 can be averted by controlled disposal
☹ However, biomass-based production can potentially compete with food security, requiring cautious auditing of supply chains	☹ Potential for systematic accumulation of brominated flame retardants in ecosystems (Domínguez et al., 2010) and human tissues (European Food Safety Authority [EFSA], 2022; Weijs et al., 2015)			☹ Health risks (SC4) can occur if retardants leach out in product use	

(*Continued*)

TABLE 5 (*Continued*)

Life-cycle stages					
Raw materials acquisition	Additive production	Packaging and distribution	Compounding/converting	Product use/maintenance	Post-use management
Timber used in window profiles					
☹ Nonsustainable timber extraction can damage ecosystems including aquifer (SC3), mobilize sequestered carbon (SC2), and impinge on forest-dweller rights (SC4)				☹ Periodic inputs of biocidal timber treatment are required to extend inherently biodegradable product life, or wood product requires frequent replacement, both combining to produce a shorter service life	☹ Biocidal timber treatment can inhibit recycling at end-of-life, leading to linear resource use
☺ Sustainable forestry practices can limit ecological harm and potentially be carbon neutral and ethical				☺ Well-manufactured wooden window profiles provide comfort, soundproofing, and thermal insulation	
Use of mined cobalt, for example, in the production of some solar panels					
☹ Cobalt is a scarce metal that may systematically accumulate in nature during incautious extraction and purification (SC1), and open cast mining is damaging to ecosystems including groundwater (SC3)				☺ Solar panel applications using mined cobalt can be long-lived yield high societal value (SC4) with significant savings in carbon emissions relative to fossil fuel-based generation (SC2)	☹ Cobalt is a scarce metal that may systematically accumulate in nature with incautious disposal
☹ Cobalt mining in some regions is associated with human rights abuses, funding repressive regimes, and creating geopolitical inequities (e.g., Karlsson & Zimmer, 2020; Sovacool, 2019)					↑ Controlled-loop recovery can retain material value and avert health risks (SC4) as well as pollution (SC1)

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(LCSA) approach with recommendations for its further development. Sala et al. (2013) observed that life-cycle thinking was covered only in a fragmented manner by discrete environmental, economic, and social "pillars" including life-cycle assessment (LCA), life-cycle costing, and social LCA (sLCA) that, through lack of integration, fail to deal with the complexity of sustainable development from "cradle to grave." Ny et al. (2008) also recognized that sustainable management of materials and products requires continuous and simultaneous evaluation of numerous complex social, ecological, and economic factors, noting that LCAs often also lack broader contextualization in sustainability principles as well as introducing difficult trade-offs. Troullaki et al. (2021) note that sustainability science (SS) has hardly permeated the applied field of sustainability assessment (SA), citing LCSA as the most commonly studied SA framework although, as currently framed and applied, LCSA does not meet SS requirements. Keller et al. (2015) found that a practical application of LCSA in *ex ante* decision support required additional features and flexibility for focus on relevant sustainability aspects and the derivation of concrete conclusions and recommendations as part of an extended "integrated life-cycle sustainability assessment" (ILCSA). Ny et al. (2008) recommended integration of the sustainability principles (System Conditions) of TNS into LCA as "strategic life-cycle management"; this subsequently evolved into the SLCA approach from which ASF was adapted specifically to address the sustainable use of chemical substances (see Supporting Information: #02). In essence, the SLCA/ASF approach embeds these extensions of LCA to embrace wider dimensions of sustainable development addressed through multiple questions addressing both (negative) impacts and (positive) innovations and contributions to sustainability across final product life and end-of-life, ASF doing so specifically for assessment of the use of chemicals.

Positively, all evaluated assessment systems were judged as founded on scientific principles. A robust basis in scientific principles ensures resilience in the face of shifting public opinion, supporting defensible and comparable investment decisions and innovation relevant across materials, applications, and regions (Johnston et al., 2007). It is concerning that practical implementation of the only statutory assessment system assessed, EU REACH, is substantially based on intrinsic properties of chemicals across its four constituent processes (Registration, Evaluation, Authorisation, and Restriction), with socioeconomic considerations only subsequently coming into play significantly when substances are listed for potential substitution. EU REACH also does not address sustainable use of substances across the societal life cycles of products into which substances are incorporated in the context of wider dimensions of sustainability, including contributions to the meeting of human needs. The analysis in this article suggests that most of the evaluated assessment systems are misleading if assumed to reflect sustainability credentials on a systemic basis.

Measuring positive contributions to sustainability is important

Of all the assessment systems addressed in this study, only ASF addressed the contributions of the use of chemicals to meeting human needs. These are addressed by responses to the four "progress questions" for each ASF sustainability principle and/or life-cycle stage. Although recognition of the positive contributions of chemical use to the meeting of human needs across product life cycles constitutes a key aspect of sustainable development, recognition of positive contributions often remains overlooked (Everard & Longhurst, 2018). The functional contributions of the use of substances across life-cycle stages to facets such as durability, low maintenance requirements, and recyclability are all highly germane to addressing human needs in the safest and most materially efficient manner. The example of stabilizer additives to PVC (see Table 4) demonstrates how the use of these and similar substances can extend human utility per unit resource by enhancing product durability and service life while reducing or eliminating maintenance inputs in the use phase, with innovations facilitating product adaptability and recyclability. Assessment systems founded more narrowly on potential hazard informed by the intrinsic properties of substances addressed in effect only assess potential bad outcomes for ecosystems and people, rather than balancing negative and positive aspects of operational risk informed by the likelihood of exposure.

Assessment systems vary in their transparency and scope to drive innovation

Although all the 17 selected assessment systems are based on scientific principles, only five were found to be open access and free to use (albeit with potential commercial guidance and external auditing aiding their more effective application). If not transparent in operation, assessment systems including "black box" methods may evade wider scrutiny and may also obscure focal aspects for innovation for sustainability. Also, some assessment systems were found to be explicitly aimed at material substitution, rather than highlighting areas of innovation of supply-chain management, chemistry, and manufacturing processes, and material management throughout the product life cycle.

It is also important for comparability of the use of different substances that assessment systems are relevant across different materials. Only two of the assessed assessment systems (ECHA Plastic Additives Initiative and material flow cost accounting [MFCA]) were not considered germane to all materials. Everard (2020) also concluded that the five TNS Sustainable Challenges for PVC founded on life-cycle analysis against the four TNS System Conditions, a substantive part of the conceptual basis of ASF, had generic relevance across alternative materials in common PVC applications including timber and/or forest-based product window profiles, ductile iron water pipes, and polyolefin pipes and cable insulation.

Application of ASF to a variety of materials

Issues summarized in Table 5 relating to the life cycles of a selected range of substances (stabilizer and flame-retardant additives in polymers, timber in window frames, and cobalt in solar panels) highlight the importance of context-dependence if assessment systems are to genuinely address the sustainability footprint of their use. Two ostensibly identical molecules produced by supply chains with differing ethical and environmental scrutiny, from mined or biologically based resources and using different manufacturing processes, can vary substantially in positive and negative profiles. Inputs throughout the life-cycle chain, for example of energy from different sources at all life stages and of biocidal preservative and other materials used for maintenance in product life, as well as shipping methods, waste control, and the fate of products into which they are embedded at end-of-life further differentiate the overall sustainability profile.

It is therefore important that ASF is applied on a product-specific basis. Generic assessments of molecule type overlooking this more nuanced assessment of sustainability performance in a whole life-cycle context can be misleading. Product-specific ASF analysis also highlights "hot spots" for innovation, whether by chemical manufacturers and their supply chains or others in the value chain from maintenance companies to recycling or disposal operations, to enhance the potential for sustainable use of substances within the products into which they are integrated (Everard & Blume, 2019).

Scrutinizing life-cycle elements assessed against broader sustainability principles also highlights that no material type is inherently more or less sustainable. All the diverse selected material types demonstrate potential negative and positive profiles across product life cycles, which can be influenced by management decisions and further innovation. ASF assessment also allows material suppliers to demonstrate to their customers, in objective terms, unique and potentially competitive sustainability performance against a transparent, science-based framework.

A proactive approach to sustainable development based on common principles

Increasing human demands subsisting on a declining natural resource base dictate that sustainability pressures will impinge progressively on and shape supply-chain security, potential liabilities, regulation, customer demand, and other economic considerations, and consequently decision-making about material choice. The Natural Step approach of backcasting from science-based sustainability principles, as embedded in ASF, represents a more strategic and beneficial approach than reacting to issues only once they manifest in scientific, public, NGO, customer, and government consciousness and response, often leading only to short-term substitution decisions rather than systemic innovation in sourcing, chemistry and manufacturing processes, and life-cycle handling of products. Founding material manufacturing and use decisions proactively on science-based sustainability criteria therefore makes strategic sense and, by implication, sound business judgment.

The purpose of this article is not to denigrate any chemical assessment approach, because all have value in the context of the design principles for which they are established. However, not all are designed for transparent and science-based assessment of the sustainability "footprint" of the use of substances throughout the societal life cycles of the products into which they are incorporated, addressed on a risk basis, and including positive contributions to the meeting of human needs. The illustrative application of these principles to the use of a spectrum of material types highlights how the ASF approach allows assessment of the sustainability footprint generically across material types, highlighting potentially positive as well as negative sustainability implications covering a range of sustainable development principles and life-cycle stages. The principles underpinning the ASF approach thereby provide a framework for bespoke sustainability assessment and reporting of the use of substances, and a basis for innovation to increase sustainability.

The current regulatory environment largely overlooks life-cycle risk, wider dimensions of sustainability, and positive contributions to meeting human needs in an integrated manner. There is a consequent need to evolve regulatory thinking to assess sustainable use, progressing beyond more easily implemented but nonetheless simplistic approaches based substantially on intrinsic properties. This is necessary to propel society and commercial innovation into a systemic approach to sustainable development grounded in optimally efficient and safe means to meet human needs, consistent with addressing the UN Sustainable Development Goals. Common sustainability principles must also be applied to management of international supply chains, through regulation and/or voluntary controls implemented by value chains, such that products made inexpensively through less sustainable means and uses do not undermine those developed with investment in more responsible production.

Additional research and implementation needs

Further research is necessary to assess the sustainability footprint of more substances, testing the relevance and value of the ASF approach to industry, regulators, and along whole value chains including benefits to society as a whole. System innovation is essential to achieve fundamental changes in both social dimensions and technical dimensions and, importantly, the relations between them, noting that realization of sustainable chemistry "…requires the transformation of value chains as well as institutional and financial structures…" (Blum et al., 2017, p. 98). Consequently, this further research can help sectors of society beyond manufacturing companies—specifiers, waste and recycling, regulators, and so forth—adapt this knowledge to progress and accelerate their practical engagement with sustainable development. Implementation of these approaches can help them avoid future problems that include, for example, investment in materials considered safe today that may be revealed as problematic in future or overlooking the benefits of recycling to achieve more sustainable "circular economy" objectives. Scientifically informed communication about sustainability objectives can thereby drive innovation of increasingly sustainable solutions at all points along value chains.

Embedding these principles in everyday practice, migrating beyond assessment systems and regulations more narrowly framed by intrinsic chemical properties, is essential to make robust judgments about the sustainable use of chemicals, necessary innovations, and investments, and their objective contributions to meeting human needs. The underpinning principles need to be applied across material types and along increasingly global value chains if sustainability is to be achieved. In short, there is a need for a genuine and transparent "level playing field" for assessment of the use of all materials used by society, including their differing global supply chains, if progress toward sustainability is to be achieved, rather than naïve assumptions about "good" and "bad" materials devoid of life-cycle context and overlooking necessary innovations.

CONCLUSIONS

- Available chemical assessment systems differ in their framing characteristics. All chemical assessment systems are designed for specific purposes; extrapolating beyond those purposes may lead to misleading conclusions. Few assessment systems used in the chemicals sector are systemically framed around risk grounded in sustainability principles across whole product life cycles, including explicit linkage to social and economic contexts, providing a basis for backcasting from clear sustainability goals.
- A robust and transparent basis in science is important. This ensures that assessment systems are not affected by shifting public opinion, that findings are objective, neutral, and comparable across applications, can drive innovation through highlighting "sustainability hot spots," and can support robustly founded communication to external audiences.
- Measuring positive contributions to meet human needs sustainably is important for assessment systems to be genuinely attuned to sustainability assessment and innovation. Of the assessment systems examined, only ASF considered the positive contributions of the use of substances to the meeting of human needs across whole product life cycles.
- Generic relevance of assessment systems across chemical applications is important for common and objective assessment of the sustainability performance of the use of materials on a level playing field. Regulatory evolution is required to embed this into societal norms, embracing not only wider sustainability principles but also applying them across global value chains.

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The author is the sole author of this curiosity-led research noting that the tendency in chemical (and other) assessment schemes often fails to take a fully systemic approach, and that there is currently no genuinely level playing field for assessment of the use of additive chemical substances (selected as the author has some knowledge of them but also as they seem to have been subject to a disproportionately high degree of scrutiny that, prejudicially, is not then applied to other alternative substances). The author has not received funding from research institutions or interested companies.

AUTHOR CONTRIBUTION

This article is a sole research output from the author. **Mark Everard**: Conceptualization; data curation and formal analysis; investigation; methodology; validation; visualization; writing—original draft preparation; and writing—review and editing.

CONFLICT OF INTEREST

The author declares no conflict of interest.

DATA AVAILABILITY STATEMENT

All relevant assessment data—qualitative rather than quantitative—are included in the Supporting information.

SUPPORTING INFORMATION

Spreadsheet documenting assessment of chemical assessment systems against a range of sustainability criteria. Supplementary word file providing a more detailed background to ASF.

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ANNEX A: THEORETICAL RISK ASSESSMENT AND ITS PRACTICAL ACHIEVEMENT

Some chemical assessment approaches are based entirely on hazard criteria. Some others are described as taking a risk-based approach but are initially founded on assessment of the intrinsic properties of substances with socioeconomic considerations only later in implementation.

Although EU REACH regulations refer to risk in terms of chemical evaluation aimed at improving protection of human health and the environment (European Chemicals Agency [ECHA], 2022), the principal definitions of REACH emphasize a foundation in "intrinsic properties" such as (author's emphasis in bold) the European Commission (2006) "REACH (European Commission [EC], 2008) aims to improve the protection of human health and the environment through the better and earlier identification of the **intrinsic properties of chemical substances**…," the UK Health and Safety Executive's International Uniform ChemicaL Information Database (IUCLID) intended to implement REACH principles (HSE, 2022) also citing a basis in "…better and earlier identification of the **intrinsic properties of chemical substances**", and the European Chemicals Agency (ECHA; 2011) *Guidance on information requirements and chemical safety assessment—Chapter R.2: Framework for generation of information on* ***intrinsic properties***.

Framing chemical assessments in ECHA (2022) guidance initially focus principally on the intrinsic properties of substances leading through the Registration, Evaluation, Authorisation, and Restriction phases. Only once restrictions or inclusion in annexes setting time limits on authorization have been established are wider socioeconomic considerations applied when considering substitution by other substances.