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Full length article

A Chemical Element Sustainability Index

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ABSTRACT

As product development becomes increasingly complex, the demand for the earth's mineral ores increases and with it, the challenge to achieve global "sustainability". Chemical elements are the building blocks of natural resources which are sourced from across the planet to manufacture globally traded goods. While global technological, social and economic progress accelerates, evaluating the sustainability of these building blocks remains a challenge. Numerous methodologies to evaluate sustainability exist but most rely on high levels of data collection. In this paper, a methodology is presented within a multi-criteria decision analysis and composite indicator framework with the aim of rapidly and comprehensively estimating the sustainability of a chemical element. The framework is based on triple bottom line principles; the environment, economy and society, to measure the sustainability of 59 chemical elements. The output, the chemical element sustainability index (CESI), is a single value supported by the aggregation of the Human Development Index, Global Warming Potential, and National Economic Importance indicators, derived through a rigorous and systematic selection process. Recycling rate is employed within the framework as a control variable given its importance as a sustainability strategy. The results show that the greater the Human Development Index, National Economic Importance and Recycling Rate, and the lower the Global Warming Potential, the more sustainable the chemical element is, and vice-versa. The CESI was validated using three representative piezoelectric materials as a case study. The framework presented is useful for product designers, policy makers and educational bodies, to support decision making towards sustainable production and consumption.

Abbreviations

CESI	Chemical Element Sustainability Index
GDP	Gross Domestic Product
GII	Global Innovation Index
GWP	Global Warming Potential
HDI	Human Development Index
InvGWP	Inverse Global Warming Potential
KNN	Potassium sodium niobate
LCA	Life Cycle Assessment
NEI	National Economic Importance
NBT	Sodium bismuth titanate
OECD	Organisation for Economic Co-operation and Development
PCA	Principal Component Analysis
PGM	Platinum Group Metals

PPI	Policy Perception Index
ProdSI	Product Sustainability Index
PZT	Lead zirconate titanate
REE	Rare Earth Element
RR	Recycling Rate
SDG	Sustainable Development Goals
SI	Supplementary Information
USGS	United States Geological Survey

1. Introduction

Whilst different interpretations of sustainability have been developed, the interconnected relationship between society, the environment and economics is often cited (Sales et al., 2006; Griggs et al., 2013). Global sustainability requires a complete transformation in the way we

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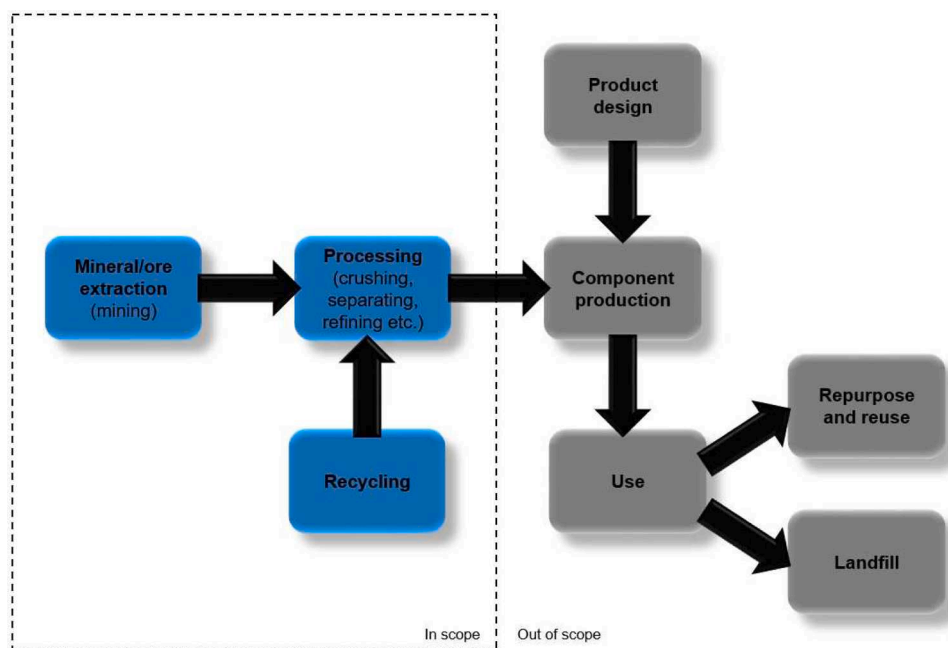


Figure 1. The scope of the Chemical Element Sustainability Index includes mineral/ore extraction, processing and the recycling phases of production to aid decision making at the product design stage. Component production, use and other end of life management strategies are out of scope.

live (Elmqvist et al., 2019), including a reduction in the consumption of natural resources, highlighted in the United Nation's Sustainable Development Goal (SDG) #12, *responsible production and consumption* (Haberl et al., 2019). Accordingly, a wide array of research has been conducted looking into different aspects that can encourage responsible production and consumption. For instance, Ku and Hung (2014) considered the management of raw materials supply risks, classifying materials into critical, near-critical and non-critical and concluding that obtaining lasting solutions to these material criticality challenges will require industries and stakeholders to cooperate with each other across the entire supply and value chain of the materials. In their report on critical materials strategy, the US Department of Energy (Bauer et al., 2010) echoed similar views whilst examining strategies to combat vulnerability to supply disruptions and geopolitical uncertainty. Graedel et al. (2011), in an attempt to improve the sustainability of metals whilst managing criticality, investigated the recycling rates of 60 metals and proposed different recycling metrics and discussion on the potentials of different recycling techniques and an estimation of end-of-life recycling rates at the global level.

Sustainability within global material supply chains is becoming increasingly important (Grey and Tarascon, 2016) especially where it presents a risk to the environment and society (Sonter et al., 2017; van den Brink et al., 2019). Global consumption of materials increased from 87 billion tons in 2015 to 92.1 billion tons in 2017, in line with economic development (Sustainable Development Goals Knowledge Platform; Henckens et al., 2014). However, while policies are in place with the view to reduce the complexity of recycling at the end of life of a product (European Commission, 2011), the number of materials used in the production of a mobile phone, for example, has increased from twelve to sixty in the last fifteen years (Sonter et al., 2017). This suggests that product development is becoming increasingly complex, with a corresponding increase in demand for the earth's mineral ores, hampering progress towards attaining global sustainability.

To address these challenges, an understanding of the sustainability

profile of chemical elements i.e. the building blocks of natural resources which are sourced from across the planet to manufacture goods that are traded globally, is pertinent. However, as global technological, social and economic progress accelerates, the evaluation of the sustainability of these building blocks remains a challenge. One of the main challenges pertains to the proliferations of different methodologies for measuring sustainability, characterised by a reliance on high levels of data collection and disaggregated outputs that hinder understanding and easy interpretation, thereby creating confusion amongst stakeholders. As such, a robust method that can rapidly and comprehensively estimate the sustainability of a chemical element is required. Hanson (2003) suggested that the "holy grail" of sustainability measurement would be a single accepted indicator which, according to Elkington's (1994) concept of the triple bottom line, requires a balanced view of economic, environmental and social aspects.

With this in mind, we present the Chemical Element Sustainability Index (CESI), a robust methodology to estimate the sustainability of different chemical elements. The CESI adopts quantitative methods within a multi-criteria decision analysis and composite indicator framework, to assess the sustainability of 59 chemical elements, including platinum group metals (PGMs) and rare earth elements (REEs), based on the triple bottom line framework. An outline of the construction of the CESI framework, developed using a thorough and methodical selection process based on criteria informed by an extant literature review, is presented. The final framework is comprised of four, equally weighted and geometrically aggregated indicators namely the (i) Human Development Index (HDI), to measure the social pillar of sustainability; (ii) Global Warming Potential (GWP), which represents the environmental pillar of sustainability; (iii) National Economic Importance (NEI), which is a function of the economic aspects of sustainability; and (iv) Recycling Rate (RR). Although RR is not directly linked to the triple bottom line, it is employed within the overall framework as a control variable to better understand the elements under consideration given its importance as a sustainability strategy in the

current climate of resource efficiency and circular economy (Graedel et al., 2011). Overall, for a chemical element to have a high sustainability result, countries producing the element should aim to have a high HDI, NEI and RR and look to reduce the GWP impact of the element itself. The single value result attributed to each of the chemical elements measured is further fully disaggregated to indicate the percentage contribution of each underlying indicator to the final result, based on in-depth analysis of 2014 and 2015 datasets, thus allowing for transparency and visibility of the individual triple bottom line attributes of each element.

A case study is outlined through the application of the CESI to three piezoelectric materials, lead zirconate titanate (PZT), potassium sodium niobate (KNN) and sodium bismuth titanate (NBT) which had previously been ranked based on their environmental profiles using comparative life cycle assessments (Ibn-Mohammed et al., 2016; 2017; 2018). The case study serves to estimate the average sustainability impact of each piezoelectric material and their sustainability hotspots, thereby forming the basis for the validation of the CESI framework. The CESI is useful for product designers, policy makers and educational bodies, to support decision making towards sustainable production and consumption. At the time of submission, later elemental production datasets were available, though as the aim of this journal article is to demonstrate the methodology applied to construct the CESI and the initial results of the framework, the presentation based on 2014 and 2015 results is deemed appropriate.

Considering the above, this manuscript is structured as follows. Section 2 summarizes the materials and methods employed in the development of the CESI. The results of; the CESI, fully disaggregated indicator contributions, trend analysis over an 11-year period, uncertainty and sensitivity analysis, and links to other indicators, are discussed in Section 3. Section 4 discusses the verification and validation of the CESI using representative piezoelectric materials as a case study and finally, conclusion is drawn in Section 5, where an overview of the findings is provided, the limitations of the index are discussed and future related research is outlined.

2. Materials and Methods

This study builds a composite indicator to calculate the sustainability of a chemical element based on the theory of the triple bottom line. The methodological steps required for the construction of the CESI were provided by (Nardo et al., 2008) and supported by concepts from published literature and other highly cited indices.

2.1. Construction of the Theoretical Framework

The theoretical framework of the CESI is based around its fundamental aim: *to assess the sustainability of a chemical element*. It applies the theory of sustainability with respect to the triple bottom line and its symbiotic nature, where a change in one of the three pillars, may lead to a change in another (British Standards Institution, 2011). It provides policy makers, academics, industry and the public with the information required to aid their decision making with respect to product development, policy making and consumer trends (Liu et al., 2019). The scope of the CESI, shown in Figure 1, addresses mining, processing and recycling; product design production, use and other end of life scenarios are out of scope.

2.2. Index development

Secondary data was required in the construction of the CESI due to

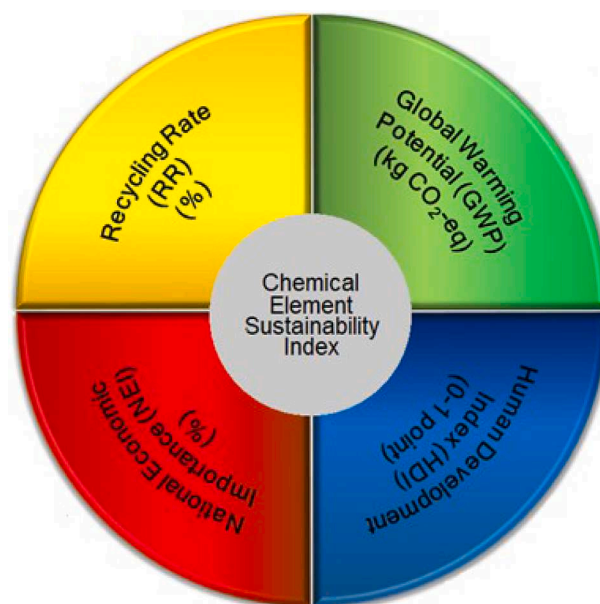


Figure 2. The Chemical Element Sustainability Index Framework is shown; the Human Development Index (sourced from the Human Development Report), the Global Warming Potential (sourced from the CML 2001 environmental impact category methodology), the Recycling Rate and the National Economic Importance (both source from the United States Geological Survey) are normalised, equally weighted and aggregated using a geometric aggregation methodology to provide a single quantitative measure of sustainability.

the wide ranging and complex supply chains associated with the chemical element extraction process. Indicator selection took the form of a detailed literature review to understand which indicators have previously been used and a selection criteria matrix was used (Kuhndt et al., 2002; Collen et al., 2009; Long et al., 2016), outlined in Table S1, to disregard indicators that did not fit the scope or aim of the CESI. The data characteristics and quality of each of the chosen indicators is summarised in the Table S2; the procedures relating to the management of missing data are provided in the SI.

Principal Component Analysis (PCA) was employed following the completion of the indicator selection process. PCA is an accessible, low-cost methodology, yielding a manageable dataset based on the underlying structure of the original data and was used to test three imputation methodologies (case deletion, average and geographic imputation) (Nardo et al., 2008). The process identifies common dimensions which may underpin the studied datasets and therefore, variance that is shared with other indicators in the dataset (common variance) is required. This methodology was applied to each dataset according to the chosen imputation methodology, for both 2014 and 2015, to determine if an underlying structure was present within the chosen indicators. The results of the PCA are shown in Appendix A, the SI and discussed in section 3.1, leading to the construction of the CESI Framework, shown in Figure 2.

The indicators were then normalised according to the procedure outlined in the SI and equal weighting was applied to each of the underlying indicators within the CESI framework. Geometric aggregation of the indicators was chosen (equation 1) to ensure that the beneficial result of one underlying indicator does not fully compensate for the poor result of another. This also echoes the interdependence of the concept of sustainability in that a change in one of the three pillars, may result in a change in another.

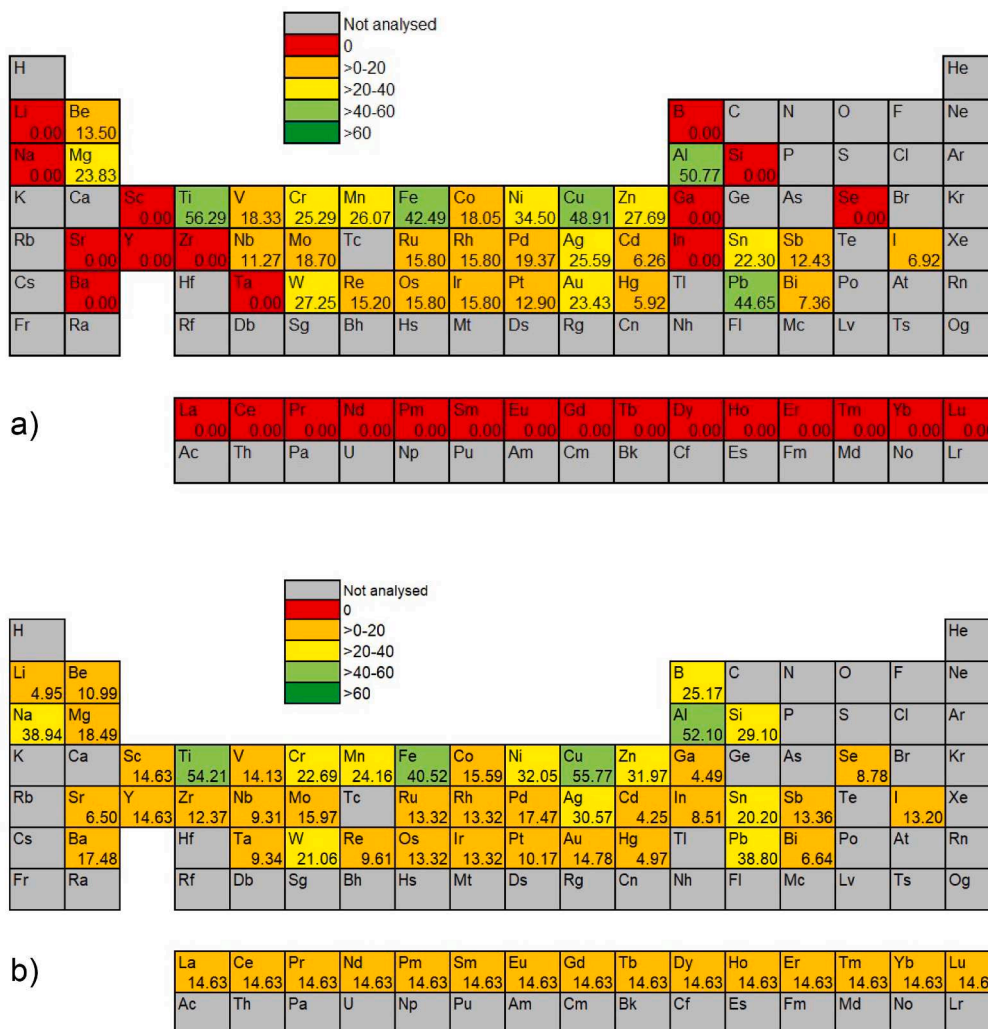


Figure 4. Colour coded periodic tables to visualise the a) 2015 Chemical Element Sustainability Index (CESI) result; b) 2015 CESI result excluding the recycling rate indicator from the assessment.

assigned to each input factor, $X_i, i = 1, 2, \dots, k$, these are detailed in the SI.

In the sensitivity analysis, the sources of uncertainty were tested to determine their impact on the CESI result for 2014 and 2015. The CESI was calculated according to the requirements of each individual input factor (X_1 to X_6). To complete the uncertainty analysis, a Monte Carlo Simulation, using random inputs to understand the behaviour of a complex system, was used to assess input factors X_1, X_2-1 and X_2-3, X_4, X_5 and X_6 . 10,000 random combinations of input factors were generated for each chemical element and for each random combination, the CESI model was evaluated.

3. Results and discussion

3.1. CESI theoretical framework

The CESI theoretical framework shown in Figure 2 is the result of a rigorous and systematic selection process (Table S1) that involved the identification of relevant indicators from a larger set of potential indicators. This highlighted the Human Development Index (HDI), the Policy Perception Index (PPI), the Global Innovation Index (GII), the Global Warming Potential (GWP), the National Economic Importance (NEI) and the Recycling Rate (RR) as applicable indicators. Using the selection criteria matrix, other indicators identified during the literature review were discarded based on duplication, relevance and accessibility.

Further robust analysis in the form of PCA was then used to

determine if an underlying structure was present within the chosen indicators. The component matrices produced by the PCA for the 2014 and 2015 indicators, shown in Table A.4, outline the component loadings for each indicator in line with the three components that show the most variance in the dataset. High and moderate loadings are considered to be those over 0.5 and therefore it can be said that, independent of the year, component 1 is represented by the HDI, PPI and GII indicators. Component 2 accounts for the RR and NEI indicators and the InvGWP indicator is represented in component 3.

The rotated component matrices for 2014 and 2015, shown in Table A.5, were produced to provide results that are more interpretable than those provided by the component matrix. The “varimax” rotation technique was applied to load a smaller number of variables, highly onto each component. The results of the “varimax” rotation mirror the results of the component matrices for each component across both years i.e. component 1 is represented by the HDI, PPI and GII indicators; component 2 accounts for the RR and NEI indicators and the InvGWP indicator is represented in component 3.

The PCA indicates that the six original indicators can be characterised by three principal components, independent of imputation methodology. The HDI, PPI and GII are represented by component 1, of which the HDI has the highest loading; the NEI and RR fall within the constructs of component 2, where the RR has the highest loading and the InvGWP is the only indicator within component 3.

Accordingly, the results of the PCA led to a CESI framework based on

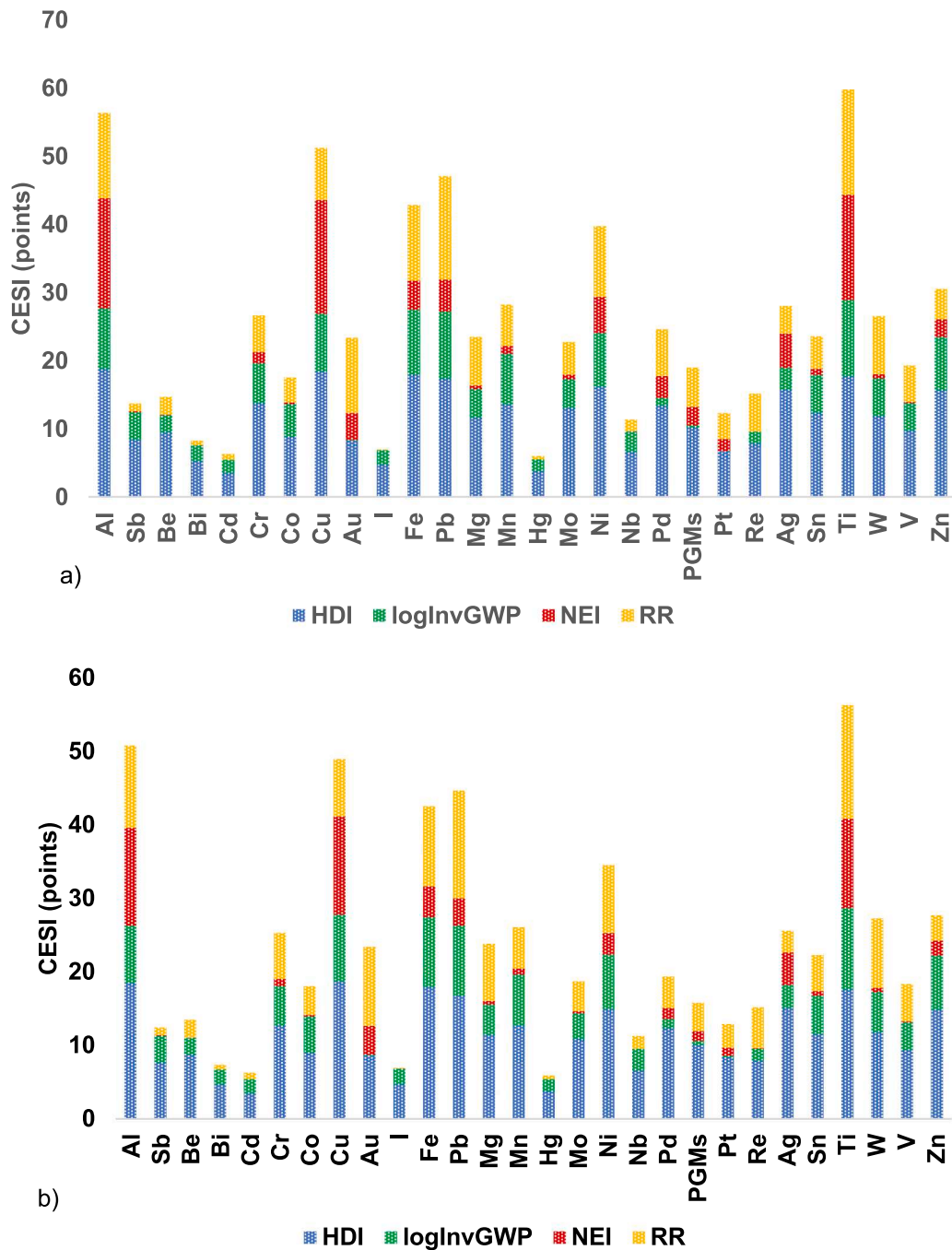


Figure 5. Decomposition of the a) 2014 and b) 2015 Chemical Element Sustainability Index (CESI) result into the four underlying indicators to show their percentage contribution to the CESI result allowing for further analysis of the final result.

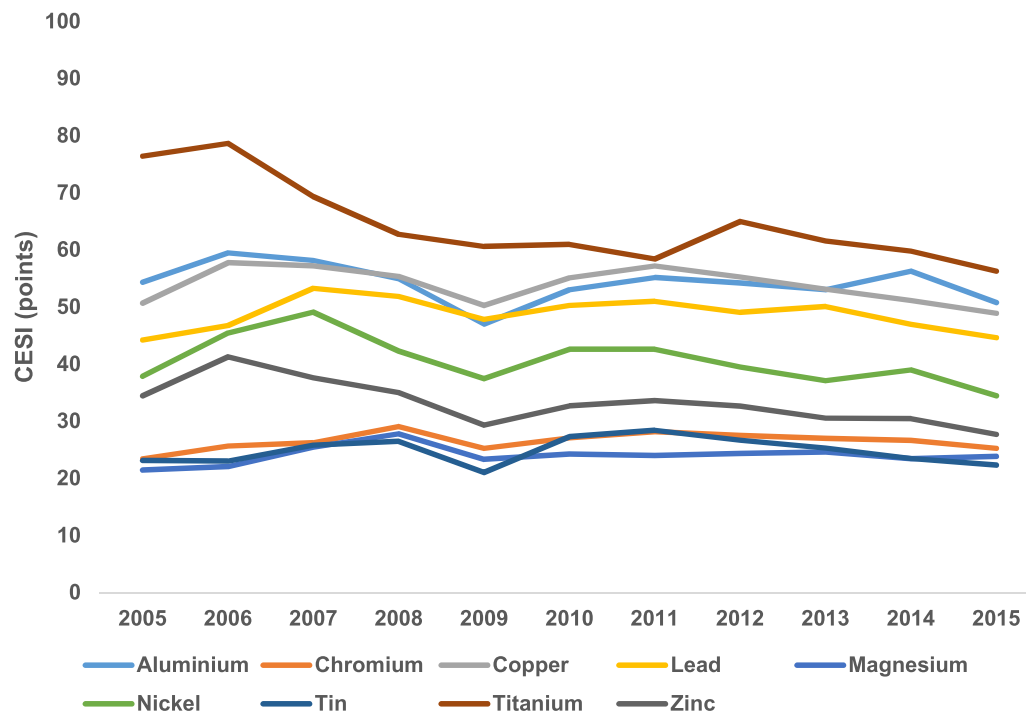


Figure 6. The CESI result was trended for aluminium, chromium, copper, lead, magnesium, nickel, tin, titanium and zinc from 2005 to 2015 to determine how the sustainability of these chemical elements has changed during this time period.

a single tier arrangement of the four individual indicators. This addresses the multidimensional phenomenon of sustainability according to the triple bottom line, through the aggregation of the GWP, NEI and HDI. The incorporation of the recycling rate (RR) is essential to acknowledge the importance of recycling in terms of sustainability (Reuter, 2011).

The social pillar of sustainability is captured by the HDI. The HDI, developed in 1990 by the UN and published annually, measures a country's development according to adult literacy, life expectancy and purchasing power (McGillivray, 1991; Deb, 2015). The HDI is included in this methodology to measure the social progress of the resource producing country (Graedel et al., 2012); as the social progress of the country increases, so does the sustainability of the resource, and vice-versa. The underlying indicators that support the HDI are not associated directly with resource extraction and therefore it is not possible to determine whether the production of an element in a certain country results in a higher or lower HDI, compared to the country's HDI without production of the element. The GWP captures the environmental pillar of sustainability, this data was sourced from the Ecoinvent database (Ecoinvent database) using the CML 2001 methodology. The GWP is defined as the change in global temperature caused by the emission of greenhouse gases and measured in kg CO₂-equivalent (CML 2001). The NEI captures the economic pillar of sustainability which is calculated by taking the value of the element (apparent consumption – equation 3) as a percentage of GDP; this measure fits within the scope of the CESI as it does not calculate the importance of a chemical element throughout its life cycle. Data was acquired from the USGS statistics database (USGS database) and the World Bank database for the United States (The World Bank database) and used as a proxy for global data. The USGS database was also utilised in this study as the source of the RR data (80% data availability), other potential RR sources could be utilised as outlined in Table S4, which includes a summary of the method, calculation and availability of each RR indicator data source.

If equal weighting is applied within the same sub-group of a composite indicator, double counting may occur when the indicators are highly correlated (Nardo et al., 2008). As a positive correlation exists between the NEI and RR, it is necessary to analyse this issue in more

detail as correlation does not automatically indicate causation.

The NEI is associated with production, price and gross domestic product (Graedel et al., 2012); mining and recycling ensure supply, but as metal demand increases, recycling alone cannot support the market and therefore the mining industry must endeavour to improve its social and environmental impacts (Ali et al., 2017). Price can also be affected by the RR, which has a knock-on effect on the rate of waste collection and efficiency of the recycling process. Despite this, labour intensive, small scale recycling is often not economically viable, leading to low recycling rates (Reck and Graedel, 2012). Other barriers to increased recycling rates are product design, the requirements of the recycling process and societal norms. To increase the RR, the amount of waste collected must increase, products design must favour recycling at end of life and recycling technologies must improve (Reck and Graedel, 2012). Taking these factors into consideration, despite the indicator correlation, the economic aspect of recycling is one of many issues and therefore the inclusion of both the NEI and RR in the final CESI framework is justified.

3.2. CESI results

The CESI must accurately and efficiently communicate the results to all stakeholders (Nardo et al., 2008), as such; visualisation of the results is an essential attribute of the CESI. Figures 3a and 4a show the results of the CESI following normalisation and aggregation using colour coded periodic tables for 2014 and 2015 (Butt et al., 2019; Qin et al., 2019).

In Figures 3 and 4, red indicates a result of 0 points ($CESI = 0$) i.e. not sustainable; orange indicates a result of >0 and up to 20 points ($0 < CESI \leq 20$) i.e. low sustainability, yellow indicates a result of >20 and up to 40 points ($20 < CESI \leq 40$) i.e. moderate sustainability; light green indicates a result of >40 and up to 60 points ($40 < CESI \leq 60$) i.e. high sustainability and dark green indicates a result above 60 points ($x > 60$) i.e. sustainable. Grey is used to identify those chemical elements that have not been analysed in this study due to a lack of data.

The implications of the use of the RR indicator was highlighted as potential misnomer within the CESI framework. As shown in Figures 3a and 4a, twenty-eight chemical elements are shown in red (i.e. a CESI

result of 0 points); this is caused by a RR result of 0% i.e. the chemical element is not recycled. For critical materials such as REEs and gallium, this poses a significant issue as their recycling is of paramount importance (European Commission, 2020a). A conflict could occur for materials such as sodium where abundance, and therefore short-term sustainability, is not an issue (Basile-Doelsch et al., 2005; Wong, 2019), therefore, to determine the results of the CESI without the influence of the recycling rate indicator, the CESI framework was calculated using equation 2 for both 2014 and 2015.

$$CESI = 3\sqrt{HDI \times GWP \times NEI} \times 100 \quad (2)$$

Figures 3b and 4b show the results of the CESI when the RR indicator is removed from the assessment (equation 2); using this methodology, all chemical elements have a CESI result above 0 points. Furthermore, no elements are shown to be in the >60 points colour band, irrespective the framework used.

Assessing the underlying indicators that contribute to the final CESI result provides a transparent output and will facilitate robust analysis and value based decision making. Deconstructing the CESI into its individual indicators allows further analysis of the final result to be performed (Nardo et al., 2008). Figures 5a and b show the percentage contribution of each indicator to the final CESI result and therefore, highlight the sustainability hotspots of a chemical element, i.e. the indicator with the lowest percentage contribution to the final result. Therefore, to increase the CESI result of a chemical element, effort should be concentrated into improving the sustainability hotspot.

Overall, the results show that to increase the sustainability of a chemical element a country must aim to increase their HDI, NEI and RR indicators. Furthermore, the sustainability of a chemical element will increase further if the GWP of that chemical element is reduced.

Figure 5 shows that the HDI has a high percentage contribution to the final CESI result for each chemical element, with the exception of gold, as the HDI is the indicator with the value closest to 1 following normalisation. For gold, the high RR results (100% in 2014 and 93% in 2015) leads to a higher percentage contribution of the RR than the HDI. No other indicators have an overriding contribution to the CESI result. Therefore, when aiming to increase the overall result of the CESI, resources should not be concentrated on increasing the result of the HDI as this would have little additional impact on the final result.

With the exceptions of titanium, aluminium and copper, the NEI leads to the lowest percentage contribution of the four indicators to the final CESI result. The difference in these results becomes apparent when the raw data points are compare, for example, the original NEI indicator value for titanium is approximately 0.05%, compared to only 0.00002% for cadmium.

When the RR indicator is removed from the CESI framework the NEI indicator becomes the second highest contributor to the final CESI result for a wider range of materials; aluminium, copper, gold, PGMs, silver and titanium. For gold, silver and PGMs, this is caused by a high GWP indicator value associated with each element. With respect to aluminium, copper and titanium, although the associated GWP indicator value is relatively low, following the normalisation process, it provides a lower value than the NEI indicator and therefore leads to a lower percentage contribution.

Therefore, when the sustainability hotspot relates to the NEI indicator, resources must be concentrated on this factor to increase the overall CESI result. The NEI indicator is calculated according to equation 3 and then taken as a percentage of the GDP (Graedel et al., 2012), therefore an increase in the NEI result can be achieved by increasing primary and secondary production, increasing imports and reducing exports. Furthermore, at present NEI data availability relates to the US only, therefore, this result may differ if a wider database became available. This would allow for the NEI indicator to be weight averaged against the production tonnes of each country (as per the HDI indicator), to provide a more representative result.

$$Apparent\ consumption = Primary\ refinery\ production$$

$$+ Second\ production\ (old\ scrap) + Imports$$

$$- Exports$$

$$\pm Changes\ in\ government\ and\ industry\ stocks \quad (3)$$

The GWP indicator is calculated as the change in global temperature caused by the emission of greenhouse gases (CML 2001), therefore if the sustainability hotspot relates to the GWP indicator, efforts must be concentrated in the reduction of the greenhouse gas emission related to the extraction of the element in question.

Irrespective of the year, the results of the CESI show titanium as the most sustainable chemical element. Using 2015 as an example, the CESI result of 56.29 points relates to a HDI value of 0.72, a GWP value of 1.31 kg CO₂-eq, a NEI value of 0.05% and a RR of 63%. While these values alone are not the optimal results for each category (selenium has the highest HDI value at 0.90; boron has the lowest GWP value at 0.09 kg CO₂-eq; copper has the highest NEI value at 0.0056%; gold has the highest RR at 93%), the partially compensatory nature of the geometric aggregation methodology provides this overall result. This mirrors the interconnected nature of sustainability, where a change in one of the three pillars, may lead to a change in another (British Standards Institution, 2011). When the three indicator calculation is used (equation 2), the element with the highest CESI value is copper at 55.77 points, while titanium drops to 54.21 points. As copper has a RR of 33%, when this indicator is removed from the methodology the CESI result benefits due to the partially compensatory nature of the geometric aggregation methodology. This comparison further strengthens the argument for the inclusion of the RR indicator in the CESI framework to ensure that recycling is viewed by stakeholders as a key component of sustainability.

Of those elements shown in Figures 3a and 4a in red (a CESI result of 0 points), seventeen are REEs and therefore have been assessed as one element due to the lack of data points for each individual REE. Consequently, the overall picture could improve in the future if REEs are reported separately and recycling rates are increased. This would require individual production, GWP, RR and NEI figures to be produced. When the RR indicator is excluded from the CESI calculation (as shown in Figures 3b and 4b), the results for REEs increases, as would be expected. Though due to the low percentage contribution of the remaining three indicators, this result remains relatively low.

The removal of the RR indicator results in no elements with a CESI value of 0 and the largest increase in the CESI result when the four and three indicator equations are compared is seen for sodium which increases from 0 points according to equation 1, to 38.94 points (in 2015) according to equation 2. Although the recycling of most resources is paramount for future use, the abundance of chemical elements such as sodium and silicon means that short-term sustainability is not vital (Basile-Doelsch et al., 2005; Wong, 2019). As such, a result of 0 CESI points may be misleading to the modeller. Despite this, silicon is classified as a critical material (European Commission 2020a), supporting the use of the RR in this specific case. Conversely, the CESI result for some chemical elements such as titanium, lead and iron are adversely affected by the removal of the RR indicator from the assessment methodology due to the high recycling rate of these elements.

Overall, the inclusion of the RR indicator is not only important for future chemical element availability (Reuter, 2011), but also because many of the chemical elements with an CESI result of 0 points are categorised as critical materials e.g. rare earth elements (European Commission 2020a). Nonetheless, the difference in the CESI results for each chemical element and the change in the result with respect to RR are readily visualised with these two assessment methodologies. To ensure the widest range of stakeholders can easily interoperate the CESI results, Table S15 and Figure S3 provide alternative visualisation methodologies.

Trend analysis of the CESI calculation was conducted to determine if

the sustainability of select chemical elements had changed between 2005 and 2015; [Figure 6](#). The CESI results of nine chemical elements were trended, these elements were chosen due to the high-quality data available in the USGS database relating to their recycling rate, the same data for the remaining elements was not available.

Over these 11 years, [Figure 6](#) shows that the sustainability of these chemical elements generally trends downwards for aluminium, copper, nickel, tin, titanium and zinc and a slight increase is seen in the chromium, lead and magnesium results across this period. The CESI result of titanium in 2005 was 76.40 points, compared to only 56.29 points in 2015. The NEI result decreased from 0.225% in 2006 to 0.049% in 2015, this is mirrored in the price trend of titanium over the same period. Although apparent consumption remains stable the reduction in price results in a reduced NEI value ([Metalary database](#)).

This example demonstrates how the CESI reflects the symbiotic nature of the three pillars of sustainability. The social, environmental and recycling rate of titanium remain marginally constant over this period but the economic impact has decreased and therefore the sustainability of the chemical element decreases. This is due to only partial compensatory nature of the geometric aggregation methodology.

When the raw data points of the GWP are plotted between 2005 and 2015 for these nine chemical elements, the results are seen to increase. [Memary et al. \(2012\)](#), using copper as an example, showed that carbon emissions increase as material production increases, despite efficiency improvements. To reduce the carbon emissions relating to material production, effort should be directed towards the mining and milling stages of the system ([Memary et al., 2012](#)).

Although this trend analysis shows a decrease in the sustainability of materials over time, by addressing the NEI, the sustainability of these materials will begin to increase as this is the sustainability hotspot within the system.

3.3. Uncertainty and Sensitivity Analysis

Uncertainty within a composite indicator is unavoidable; uncertainty and sensitivity analyses were therefore performed to ensure robustness ([Nardo et al., 2008](#)). Six potential sources of uncertainty were tested; imputation of data, the normalisation and aggregation methodologies, indicator exclusion, indicator substitution and the RR data source. Probability distribution functions were allocated to each input factor, X_i , $i = 1, 2, \dots, k$, these are summarised in the Tables S8-S9 and S11-S14.

The sensitivity analysis shows that the chosen imputation methodology provides a low level of uncertainty to the results due to the high percentage availability of the HDI. Sensitivity in the normalisation methodology is related to those chemical elements with extreme values within the dataset. The aggregation methodology provides a wide range of results depending on which methodology is applied. Excluding the NEI from the CESI leads to the highest level of uncertainty in the results and high variance in the result is seen in those chemical elements with extreme values across one or more of the four indicators. When the HDI was substituted for the PPI or GII, the CESI result reduced for most chemical elements, although the use of the PPI leads to a higher result than the GII overall. Sensitivity in the chosen RR source is high due to the inconsistency of the data collection methodologies, highlighting the necessity of consistent global data collection. Accurate implementation of SDG #12.5.1, the collection of national recycling rates ([Sustainable Development Goals Knowledge Platform](#)), will provide a robust global RR average and therefore, reduce the uncertainty of the CESI result.

With respect to the uncertainty analysis, in 2014 and 2015, limited variation between the original CESI result and the mean of the Monte Carlo Simulation results are observed. The largest variation is associated with the chemical element with an original CESI value of 0 points when the RR is removed from the calculation. Furthermore, extreme values of one or more of the input factors also leads to a high variation in the results. This result highlights the necessity to ensure that the normalisation methodology employed in the construction of a composite

indicator provides values that are scaled appropriately and therefore are comparable. Employing uncertainty and sensitivity analysis in the construction of the CESI contributes to a soundly structured framework and aids in its robustness and reliability ([Nardo et al., 2008](#)).

3.4. Links to other indicators

3.4.1. Composite indicators for sustainability assessment

A large number of composite indicators have been developed in recent years. Of those relating to materials and products, the Product Sustainability Index (ProdSI) ([Shuaib et al., 2014](#)) is of note for comparison to the CESI. The ProdSI employs a four tier structure, broken down into economic, environment and society sub-indices to determine the sustainability of a product throughout its life cycle. In total, to complete the ProdSI calculation, data is required for 19 economic indicators, 51 environmental indicators and 18 social indicators. Different normalisation techniques are employed according to the characteristics of the indicator. The normalised indicators are then weighted and aggregated using a bottom-up aggregation technique ([Shuaib et al., 2014](#)). The ProdSI and CESI are similar in their use of indicators relating to society, economy and environment (including recycling), but the former is a company-facing index which relies heavily on data mining within a corporation for each product under investigation. By using publically available sustainability indicators, the CESI reduces the onerous task of data collection to provide a robust and reliable assessment.

3.4.2. Sustainability assessment by alternative methods

BS 8905:2011 ([British Standards Institution, 2011](#)) assesses the sustainability of materials and requires the individual calculation of each of the three aspects of sustainability. This can be achieved using life cycle assessment (LCA) to calculate the environmental impacts and life cycle costing to calculate the economic impacts. As no single overriding methodology exists for social life cycle assessment, BS 8905:2011 recommends determining social impacts using either The Global Reporting Initiative, Business in the Community or OECD Guidelines for Multinational Enterprises. By assessing the three pillars of sustainability separately and then consolidating this data into one result, this methodology does not account for the interconnected nature of the triple bottom line ([Onat et al., 2017](#)). The CESI methodology overcomes this issue by aggregating four indicators to provide a single value that assesses the sustainability of a chemical element.

The EU critical raw materials assessment ([European Commission, 2017](#)), while strictly speaking not an indicator of sustainability, has some similarities with CESI. This assessment methodology utilises the end of life recycling input rate when considering the supply risk of the material and therefore can be compared to the CESI. When comparing the results of the EU critical raw materials assessment with the CESI results, all identified critical materials score 20 points or below in agreement with the CESI calculation, with the exception of magnesium, tungsten and palladium (in 2014). In 2020, bauxite, lithium, titanium and strontium were added to the list of critical raw materials ([European Commission 2020a](#)); this result mirrors the CESI result for lithium and strontium which are below 20 points. Furthermore, while aluminium is derived from bauxite, the two materials are assessed separately by the criticality assessment and therefore, the high CESI result for aluminium mirrors the result of the criticality assessment, i.e. aluminium is not a critical material ([European Commission 2020b](#)). On the other hand, titanium has CESI scores of 59.80 (2014) and 56.29 (2015) points which shows a high level of sustainability based on the CESI framework. The material has changed from non-critical in 2017 ([European Commission, 2017](#)) to critical in 2020 ([European Commission 2020b](#)) due to a change in its economic importance and supply risk. Despite this, overall, the CESI supports the findings of the EU criticality assessment. This shows, that for the majority of chemical elements, the inclusion of the RR indicator in the CESI framework is a critical to the composite indicator to

ensure a robust result.

Using 18 social indicators, 15 environmental indicators and 11 supply risk indicators, [Kolotzek et al. \(2018\)](#) aims to assess material sustainability through environmental, social and supply risk. Their methodology provides three scores between 0-100 (where 100 relates to the most critical score and 0 relates to the least critical score), one for each risk category. The team provide a case study which measures the use of aluminium, niobium and tantalum in three different capacitor types. The results of the HDI and GWP indicator, used in the construction of the CESI, can be compared to the social and environmental risk results given by [Kolotzek et al. \(2018\)](#), furthermore the average of the three risk results can be compared to the final CESI result.

The difference between the results of the social risk and the HDI indicator lead to the largest discrepancy between the two measurement types. Using the social risk assessment methodology, aluminium has the highest risk, whereas the CESI methodology gives the highest HDI indicator value for aluminium, compared to niobium and tantalum. This discrepancy can be attributed to the higher range of social indicators utilised in the calculation of social risk, compared to the HDI indicator used for the CESI. For example, the social risk calculation takes into account issues such as working hours and health and safety, assessments that were excluded from the CESI. Despite this, due to the global dispersion of mineral extraction sites, individual site data relating to specific processes become virtually impossible to obtain and therefore this type of indicator was removed from the assessment ([Arena and Azzone, 2010](#)).

[Kolotzek et al. \(2018\)](#) calculate the environmental risk of tantalum to be 28 (out of 100), the highest of the three materials measured; this mirrors the result for tantalum using the CESI (0 points) and also the result of the comparative hybrid LCA published by the authors ([Smith et al., 2018](#)). [Smith et al. \(2018\)](#) used the hybrid LCA framework to compare the environmental impacts of multi-layered ceramic capacitors and tantalum electrolytic capacitors. The results of this study showed an overwhelming environmental impact relating to tantalum electrolytic capacitors due to the tantalum mining process, compared to multi-layered ceramic capacitors. Therefore, in the case of tantalum, the high sustainability risk given by [Kolotzek et al. \(2018\)](#), the low sustainability assessment provided by the CESI and the high environmental impact shown by [Smith et al. \(2018\)](#), shows that these three calculation methods complement each other and provide comparable results.

When the average of the environmental, social and supply risks, calculated by [Kolotzek et al. \(2018\)](#), is taken for tantalum, aluminium and niobium, the results align with the CESI. On average, the highest risk material is tantalum (47.67), followed by niobium (35.67) and then aluminium (34.34). This pattern is also observed in the CESI; tantalum (0 points), niobium (11.27 points) and aluminium (50.77 points), which again demonstrates the complementary nature of these two methodologies. Overall, a wide range of composite indicators and other methodologies have been developed to assess sustainability, but none provide a single value for the sustainability of a chemical element using a composite indicator. Consequently, it is the responsibility of the modeller to determine the most appropriate methodology to provide a robust result for their material, product or system.

4. Verification and validation of CESI

As previously highlighted, the CESI was developed with the view to provide stakeholders (e.g. materials scientists, product developers etc.) with a value to estimate how the building blocks of products affect their overall sustainability using a triple bottom line framework covering environmental (GWP, kgCO₂-eq), economic (national economic importance, %) and social (human development index) indicators. The recycling rate is employed as a control variable given its importance as a sustainability strategy. Through the application of a robust and systematic methodology, informed by ([Nardo et al., 2008](#)), the CESI provides a robust composite indicator that rapidly and efficiently evaluates

Table 1a

CESI result for NBT and the CESI result for NBT excluding the recycling rate indicator (according to [equation 2](#)).

Primary constituent	wt%	CESI 2015 (points)	CESI 2015 w/o RR (points)
Bismuth oxide	52	3.85	3.47
Sodium carbonate	12	0.00	4.63
Titanium dioxide	36	20.17	19.43
Total		24.02	27.53

Table 1b

CESI Index result for PZT and the CESI result for PZT excluding the recycling rate indicator (according to [equation 2](#)).

Primary constituent	wt%	CESI 2015 (points)	CESI 2015 w/o RR (points)
Titanium dioxide	11	6.43	6.19
Zirconium dioxide	19	0.00	2.37
Lead oxide	70	30.98	26.92
Total		37.41	35.49

Table 1c

CESI result for KNN and the CESI result for KNN excluding the recycling rate indicator (according to [equation 2](#)).

Primary constituent	wt%	CESI 2015 (points)	CESI 2015 w/o RR (points)
Potassium carbonate	18	0.00	6.95
Sodium carbonate	14	0.00	5.33
Niobium pentoxide	68	7.72	6.37
Total		7.72	18.65

the sustainability of chemical elements, highlighting hotspots (i.e. the indicator with the lowest percentage contribution – a weakest link approach), and thus offers an avenue to outline improvements.

Evaluation is generally conducted with the view to *verifying and validating* a framework, tool, or a system ([Sprague Jr and Carlson, 1982](#); [Mosqueira-Rey and Moret-Bonillo, 2000](#); [Papamichail and French, 2005](#)). Whereas, verification entails checking whether a proposed model truly represents what it is constructed for, validation is about establishing whether the model developed is a true representation of the phenomenon being modelled ([Miser, 1997](#)). As such, verification is a subset of validation; a model that has not been established in the right manner is unlikely to constitute the right model ([O'keefe and Preece, 1996](#)). In the context of CESI, the appropriateness and application of the methodological framework were thoroughly examined and justified. For instance, the methodological steps required for the construction of the CESI were based on the popular handbook on constructing composite indicators ([Nardo et al., 2008](#)) and supported by concepts from published literature and other highly cited indices. Details of the methodological steps are provided [section 2](#), containing all steps and data collection strategies for the CESI design, leading to its outputs. Nevertheless, in order to validate/verify the output of CESI based on the combinations of key elements within a class of functional materials and establish its wider applicability at the material level (i.e. a combination of different elements to form a material), a case study based on three representative piezoelectric materials namely lead zirconate titanate (PZT), sodium bismuth titanate (NBT) and potassium sodium niobate (KNN) is presented in the subsection that follow.

4.1. Case study background

The CESI was applied to three key piezoelectric materials, PZT, KNN and NBT, to estimate the average sustainability impact of each piezoelectric material and their sustainability hotspots, i.e. which of the main constituents has the highest sustainability impact. Furthermore, the

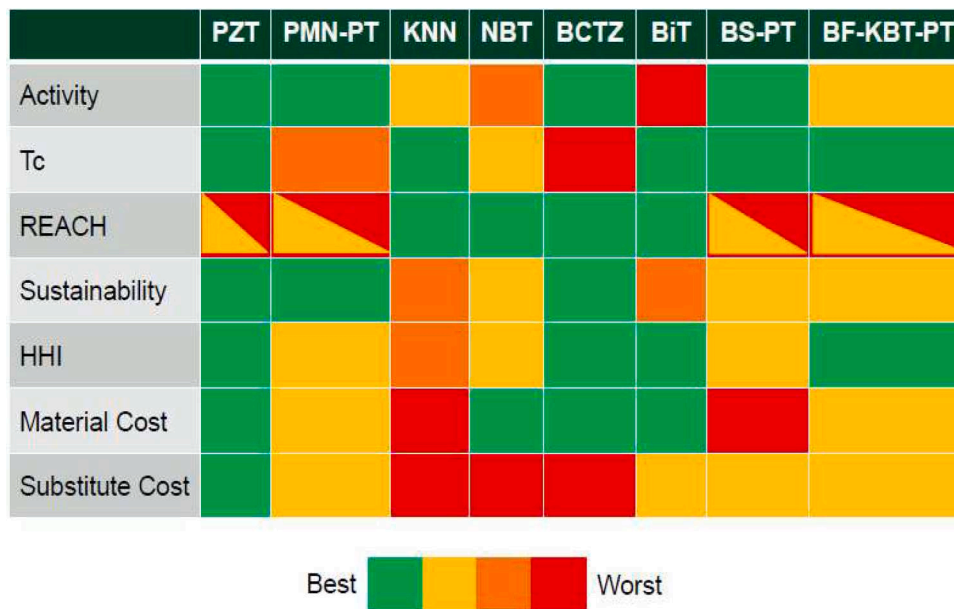


Figure 7. Risk summary of a range of piezoelectric materials, including PZT, NBT and KNN considered in this work. Adapted from Bell (2016). Registration, evaluation, authorization, and restriction of chemicals (REACH); Currie temperature (T_c); Herfindahl-Hirschman Index (HHI) – market concentration of the individual constituent elements within the piezoelectric materials (United States Department of Justice and Federal Trade Commission, 2006).

results were also assessed based on equation 2 to determine how the inclusion of the RR indicator affects the overall result. The mass of each primary constituent was determined using published literature (Ibn-Mohammed et al. 2016; 2017; 2018). The sustainability hotspot within each piezoelectric material was determined by weight averaging the mass of each constituent and multiplying the weight factor by the CESI result at the chemical element level. Due to the vast array and complexity of the compounds used in piezoelectric material production, assessment of their sustainability was carried out at the chemical element level. The sum of the weight averaged component CESI was then taken as the total sustainability impact of the material.

4.1.1. The sustainability of piezoelectric materials- A case study

As highlighted above, the CESI is also calculated using equation 2, to account for the high abundance, and therefore lower dependence on recycling of sodium. Given that CESI result is unavailable for potassium, the result for sodium was used as a proxy. These results are shown in Tables 1a – c (Ibn-Mohammed et al. 2016; 2017 2018).

As shown in Tables 1a – c, irrespective of whether the RR indicator is utilised, the piezoelectric with the highest CESI result is PZT, followed by NBT and finally KNN. The high CESI result including the RR indicator for lead and titanium (44.65 and 56.29 points respectively) contribute to the high result for PZT, though the CESI result for PZT decreases when the RR indicator is removed from the calculation due to the high recycling rates of both elements (68% for lead and 63% for titanium). As zirconium is not recycled, when the RR indicator is removed from the CESI the result increases from 0 to 12.37 points, thereby contributing to the overall CESI but remaining as the sustainability hotspot within the system.

The CESI result from KNN is dominated by the fact that sodium and potassium are not recycled, giving a CESI result of 0 points and therefore, the sustainability hotspots within the system. Furthermore, the CESI of niobium is also relatively low (11.27 points), this is dominated by a low result for the NEI indicator, and niobium constitutes 68% of the total weight of KNN. When the RR is removed from the CESI, the result for sodium (and potassium) increases to 38.94, rendering niobium as the

sustainability hotspot. This increase in the sodium CESI result is due to the partially compensatory nature of the geometric aggregation methodology which, in this case, is affected by a high NEI result for sodium.

When these CESI results are compared to other available techniques, e.g. LCA, the findings are comparable. Ibn-Mohammed et al. (2018) showed that the environmental impact of KNN is considerably higher than that of PZT and NBT over a range of different environmental impact categories, while the lowest environmental impact was seen for NBT (Ibn-Mohammed et al., 2018). Additionally, the results presented here are also validated/verified when compared to the summary risk breakdown of selected piezoelectric materials based on the work of Bell (2016) as depicted in Figure 7. As shown, using sustainability indicator as an example, KNN has the worst overall sustainability profile, followed by NBT, with PZT emerging as the most “sustainable”.

This result, as mentioned above, is due to the high CESI values of titanium and lead in PZT which outweigh those of titanium and bismuth in NBT. As the environmental impact is not the only contributing factor to the final CESI result, the NEI of niobium and RR of sodium should be increased to increase the sustainability of KNN. Overall, the case study presented indicates that PZT is the most sustainable piezoelectric material, followed by NBT and KNN as the least sustainable, in agreement with previously published comparative life cycle assessments.

5. Conclusion

This study presents the methodological construction and results of the CESI, a robust and efficient calculation for the sustainability of a chemical element based on the triple bottom line; this is the first of its kind. In this study the CESI is applied to 59 chemical elements, including platinum group metals and rare earth elements.

The results of the CESI show that those chemical elements classified as critical, e.g. REEs and silicon, have a low CESI result. This is due to the lack of recycling associated with these elements. Removing the recycling rate indicator from the assessment methodology may be relevant for those materials of high abundance but is crucial in the case of critical materials such as REEs and silicon.

The sustainability hotspots for the majority of chemical elements is the national economic importance indicator and therefore, resources must be focussed on this aspect to improve the sustainability of chemical elements. Furthermore, the application of the CESI between 2005 and 2015 has shown that material sustainability decreased due to a fall in material output and the consequential increase in the related global warming potential.

The CESI was applied to three key piezoelectric materials as a case study. The results are comparable to previously published work on their environmental impact. Attempts were made to verify and validate CESI from a technical point of view. However, to fully verify and validate the CESI, future work surrounds the application of the index to an industrial case study whilst making a comparison of the results to other available methodologies, confirming its application in a real-world setting.

In the construction of the CESI, the main limitation is data availability. A literature review identified sustainability indicators as potential candidates for the CESI but the majority of these were excluded due to the absence of available data. Those indicators with enough data to produce a meaningful result still had data gaps that had to be managed appropriately.

As described, the HDI indicator values for each country were weight averaged against the chemical element production tonnes to determine the HDI of each chemical element (as performed by Graedel et al. (2012)). To determine a truly global assessment of chemical element sustainability, it would be beneficial to be able to apply the step to the remaining indicators but this was not possible due to the dearth of individual country data for the GWP, NEI and RR data sets. Furthermore, if these datasets were available, the CESI could be calculated on a country basis, allowing for additional benchmarking between countries.

A prime example of discrepancies in data collection methodologies can be seen in the RR indicator; four different sources (European Commission, 2014; Graedel et al., 2011; Royal Society of Chemistry database; USGS database) provide three different collection methodologies which are taken from different global regions, see Table S4. This leads to inconsistent final RR indicator values and emphasises the need for a global standard on recycling rate data collection. Furthermore, this inconsistency is reflected in the results of the CESI sensitivity analysis, which shows a wide range in the CESI result when different RR indicator sources are used in the calculation, leading to potential uncertainty in the final result.

Another limitation to the CESI lies in the absence of a comparative weighting methodology to be tested by the uncertainty and sensitivity analysis. The indicator weighting methodology may provide a source of uncertainty, but this was not included in the assessment due to a lack of alternative methodologies against which to compare the equal weighting strategy, e.g. budget allocation.

Despite these limitations, through utilisation of the guidance provided by Nardo et al. (2008) throughout the construction of this framework, the level of subjectivity imparted on the result has been reduced as far as possible. Despite this, it is impossible to ensure that all uncertainty is eradicated from a composite indicator. Overall, the CESI provides a simple tool for the evaluation of the sustainability of a chemical element for decision support by product developers, policy makers and other key stakeholders.

Table A.2

Total variance explained of the case deletion imputation methodology 2014.

Component	Initial Eigenvalues			Extraction Sums of Squared Loadings			Rotation Sums of Squared Loadings		
	Total	% of Variance	Cumulative %	Total	% of Variance	Cumulative %	Total	% of Variance	Cumulative %
1	2.104	35.062	35.062	2.104	35.062	35.062	2.089	34.821	34.821
2	1.671	27.858	62.919	1.671	27.858	62.919	1.672	27.860	62.681
3	1.077	17.946	80.865	1.077	17.946	80.865	1.091	18.184	80.865
4	0.566	9.432	90.297						
5	0.433	7.219	97.516						
6	0.149	2.484	100.000						

Extraction Method: Principal Component Analysis.

Data availability

All data is available on reasonable request from the corresponding author.

Author contributions

S. C. L. Koh conceived the research, L. Smith designed and ran the model and conducted the analysis. All authors contributed to the preparation, review and editing of the manuscript.

Declaration of Competing Interest

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

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Supplementary materials

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Appendix A

Principal Component Analysis

The results for the case depletion imputation methodology for 2014 and 2015 are shown in Tables A.1-A5, the communalities are shown in Table A.1, the eigenvalues are shown in Tables A.2 (2014) and A.3 (2015), the associated scree plots are provided in Figures S1 (2014) and S2 (2015), the component matrix for both 2014 and 2015 is given in Table A.4 and the rotated component matrix for both 2014 and 2015 is given in Table A.5.

Table A.1

Communalities of the case deletion imputation methodology 2014 and 2015.

Standardised Indicator	2014		2015	
	Initial	Extraction	Initial	Extraction
Zscore(HDI)	1.000	0.912	1.000	0.883
Zscore(PPI)	1.000	0.724	1.000	0.724
Zscore(GII)	1.000	0.832	1.000	0.854
Zscore(InvGWP)	1.000	0.912	1.000	0.888
Zscore(NEI)	1.000	0.709	1.000	0.685
Zscore(RR)	1.000	0.762	1.000	0.766

Extraction Method: Principal Component Analysis.

Table A.3

Total variance explained of the case deletion imputation methodology 2015.

Component	Initial Eigenvalues			Extraction Sums of Squared Loadings			Rotation Sums of Squared Loadings		
	Total	% of Variance	Cumulative %	Total	% of Variance	Cumulative %	Total	% of Variance	Cumulative %
1	2.079	34.645	34.645	2.079	34.645	34.645	2.043	34.048	34.048
2	1.586	26.439	61.084	1.586	26.439	61.084	1.596	26.608	60.656
3	1.136	18.932	80.016	1.136	18.932	80.016	1.162	19.360	80.016
4	0.597	9.942	89.958						
5	0.414	6.901	96.859						
6	0.188	3.141	100.000						

Extraction Method: Principal Component Analysis.

Table A.4

Component matrix of the case deletion imputation methodology 2014 and 2015.

Standardised Indicator	2014 Component			2015 Component		
	1	2	3	1	2	3
Zscore(HDI)	0.951	0.076	-0.027	0.930	0.100	-0.085
Zscore(PPI)	0.592	0.480	0.378	0.595	0.411	0.449
Zscore(GII)	0.873	-0.015	-0.263	0.873	0.028	-0.302
Zscore(InvGWP)	0.042	-0.261	0.918	0.090	-0.239	0.907
Zscore(NEI)	-0.164	0.816	0.131	-0.160	0.806	0.103
Zscore(RR)	-0.238	0.838	-0.061	-0.252	0.837	-0.041

Extraction Method: Principal Component Analysis.

a. 3 components extracted.

Table A.5

Rotated component matrix of the case deletion imputation methodology 2014 and 2015.

Standardised Indicator	2014 Component			2015 Component		
	1	2	3	1	2	3
Zscore(HDI)	0.951	-0.081	0.029	0.935	-0.067	0.057
Zscore(PPI)	0.646	0.426	0.355	0.588	0.345	0.510
Zscore(GII)	0.870	-0.190	-0.198	0.898	-0.148	-0.161
Zscore(InvGWP)	-0.045	-0.137	0.944	-0.087	-0.165	0.924
Zscore(NEI)	-0.031	0.841	0.016	-0.024	0.827	0.023
Zscore(RR)	-0.091	0.849	-0.182	-0.088	0.860	-0.136

Extraction Method: Principal Component Analysis. Rotation Method: Varimax with Kaiser Normalisation.a

a. Rotation converged in 4 iterations.

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