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A predictive modelling-based material selection method for sustainable product design

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Material selection significantly affects environmental impacts and other objectives of a product design. Life cycle assessment (LCA) methods are not efficient enough for use at the early design stages to prune a design space. Material properties consist of discrete data sets, which are further complicated when LCA data are included, thus posing a significant challenge in the construction of surrogate models for prediction of all relevant behaviours and numerical optimisation. In this work, we address the unique challenges of material selection in sustainable product design in some important ways. Salient features of the robust surrogate modelling approach include achieving manageable dimensionality of LCA with a minimal loss of the important information by the consolidation of significant factors into categorised groups, as well as subsequent efficiency enhancement by a streamlined process that avoids the construction of full LCA. This approach combines efficiency of use with a mathematically rigorous representation of any pertinent objectives across a design space. To this end, we adapt a two-stage sampling approach in surrogate model construction for sustainability considerations based on a feasible approximation of a Latin Hypercube design at the first stage. The development and implementation of the method are illustrated with the aid of an automotive disc brake design, and the results are discussed in the context of robust optimal material selection in early sustainable product design.

Keywords: life cycle assessment; surrogate modelling; material selection; sustainable design

1. Introduction[1]

Selection of the optimal material, while considering objectives for sustainable design comprehensively early in a design process, can significantly improve the overall impacts of products. Ljungberg (2007) argued that material selection is one of the most important factors that affect the quest to achieve more sustainable products. Life cycle assessment (LCA) has evolved in recent years to be regarded as a credible, high fidelity measure of environmental impacts and the associated effects of any materials or processes during a product's life cycle (Finnveden et al. 2009). Other researchers found LCA, in its current form, to be unsuitable for use by designers at the early stages of a product design (Millet et al. 2007). A recent review paper (Ramani et al. 2010) and the recent National Institute of Standards and Technology workshop

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on sustainability (Rachuri et al. 2010) both identified the need for efficient early design stage adoption of sustainability objectives.

In many cases encountered in engineering design, high fidelity models are neither practical nor cost effective to construct, and approximate (or surrogate) model construction of the design space becomes necessary to enable early design stage efficiency with suitable predictability and robustness (Booker et al. 1999; Simpson et al. 2004). Hazelrigg (1999) distinguishes between descriptive and predictive models for engineering design, and advocates for the use of predictive models during early design stages that allow for reasonable assumptions and uncertainties while focusing on the needed resolution between discrete alternatives for correct decision-making. Descriptive models, that lack modelling error, should be used where more precise representations of the physical system behaviour are needed for more detailed engineering analysis. Although material selection poses unique challenges for surrogate (or predictive) model construction due to less than ideal non-uniform locations of design choice data points in the design space, some recent work, such as that by Swiler et al. (2014), provides promising techniques to construct surrogate models to find optimal design choices to solve traditional engineering design problems.

In spite of these latest developments, very few implementations yet exist of surrogate model solutions for sustainable product design. Thus, the use of surrogate models as predictive models for sustainable design remains a topic of research. Several researchers developed techniques to minimise the burdens of manual entries required by LCA software tools for every product instance. Zhou, Yin, and Hu (2009) proposed a notable possible approach to address the research gap of a lack of surrogate modelling techniques for sustainable design and the challenges with optimal material selection. Their method integrates artificial neural networks (ANNs) with genetic algorithms (GAs) for optimal material selection in consideration of mechanical, economic, and environmental properties. Sousa, Wallace, and Eisenhard (2000) developed an ANN surrogate modelling method to better streamline the LCA process and define some product groupings. More recently, Sousa and Wallace (2006) used these groupings to develop a product classification system by deployment of learning surrogate models constructed from the groupings. A recent paper by Chandrasegaran et al. (2013) on knowledge representation in product design systems summarises the current advancements in robust methods and computational tools to support early design stage decisions by rigorously taking into account attributes, alternatives, and preferences. Their work (Chandrasegaran et al. 2013) also points out that such approaches trend towards consideration and representation of sustainability attributes more broadly across the complete life cycle of a product.

To address the need for a usable surrogate modelling approach in the sustainable design of products, this paper advocates use of the mathematical rigour of a normative approach for sustainable design. Hazelrigg (2003) also asserts that a model needs to find local optimal designs and also determine which of the local neighbourhoods has the global optimal solution, and in doing so the model is only valid when it supports its conclusion that the outcome most desired by the decision-maker is the optimal. Here, when a normative approach is used, the response output of a surrogate model should approximate a given single attribute utility (SAU) function and/or a composite multi-attribute utility (MAU) function. This work builds on prior work that provides such a foundation methodology for sustainable product design (Eddy et al. 2013). This prior work includes the normative computation infrastructure to determine SAU and MAU value responses for sample data locations of the pertinent attributes over a product lifecycle.

One of the major challenges concerns the number of additional design variables related to sustainability, many of which are material related. Even material-related mechanical property variables are numerous, including yield strength, modulus, shear modulus, Poisson's ratio, mass density, coefficient of thermal expansion. The challenges for sustainability were exposed in prior work. Rydh and Sun (2005) attempted to define seventeen material groups to estimate Life Cycle Inventory (LCI) data based on weakly correlated relationships between material properties and environmental impacts. A wide variety of environmental emissions parameters affect impact attributes. Thus, a robust method is needed to mitigate the effects of numerous design variables and construct a surrogate model with adequate efficiency and valid resolution for optimal alternative selection. To this end, this work prescribes a way to extend techniques for surrogate model construction and testing to simplify and accelerate LCA execution at early design stages while maintaining the mathematical rigour of a multi-objective normative problem formulation.

The following sections introduce such a methodical approach for robust surrogate modelling for material selection in sustainable design of products (MASSDOP). Section 2 prescribes a fundamental foundation to formulate a problem by representing a sustainability-based design space. Section 3 introduces a mapping methodology for modelling. Section 4 adapts surrogate model construction and testing techniques to estimate the design space identified in the prior sections. Section 5 addresses issues related to optimisation of such a constructed surrogate model. Section 6 demonstrates how the entire methodology can be used with a case study example of the design of a disc brake for an automobile. Sections 7 and 8 discuss and summarise the results in the context of the challenges that this work aims to address.

2. Rationale for problem formulation

This section explains the basis on which the MASSDOP methodology is developed. A product lifecycle includes the five stages of: material extraction, manufacturing of components and assemblies from the materials, distribution of a finished product to the point of use, the use of the product over its lifetime, and disposition of the product or its components at the end of its usable life. At early design, a designer is faced with a tradeoff between enough accuracy to find the optimal design concept without sacrificing the efficiency needed at an early design stage. Thus, this section covers both the assumptions upon which this approach is based and some generalised direction for how it might be applied to a wide array of design instances. For example, impacts from the distribution stage can vary widely depending upon the product size and the potential for localised materials and production. For some products, the differences in such impacts between different designs are negligible, but for others they may not be.

2.1. *Material selection focus*

Prior published approaches (Devanathan et al. 2010; Gilchrist et al. 2013; Srivastava and Shu 2013) provide the means to map various functions and associated forms to associated environmental impacts. These works are valuable in that they provide insight to designers about which functions redesign should focus on to significantly reduce environmental impacts. For such a goal of main concept selection, the accuracy of the impact computation is not the concern. However, once the functional concept is selected, greater accuracy of the environmental impacts of bill of material options for that intended function and associated form can allow formulation as an optimisation problem. To bridge the gap, there is a need for a mapping methodology that focuses more closely and more precisely on the impacts of the main components for a previously determined intended use and general form of the product to achieve that function. Furthermore, the graph in Figure 1 shows, by an example of the case of machining steel or aluminium to half its mass, that the processes related to material acquisition and disposal are generally much more significant than those of a manufacturing process. This by no means suggests that impacts of manufacturing processes should not be considered at some point in a design process. However,

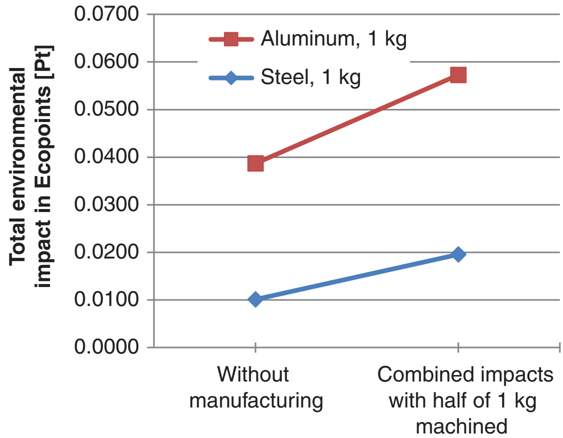

Figure 1. Example of impacts during a manufacturing stage.

to focus on the most significant impacts in the early design stages, the results in Figure 1 suggest that selection of the best bill of materials could be considered a priority for surrogate model construction.

An LCA process begins with the first step of identification of the goal and scope of a process (Scientific Applications International Corporation and Curran 2006). Here, it becomes convenient to model material alternatives for comparison on a per kilogram mass unit basis, because the extraction and end of life stages can be modelled as such in an LCA simulation. Furthermore, mass density properties are usually available for most materials and conversion to volume units can be done for all data points. This allows for a convenient consideration of the geometry of components as well as the material. It can be especially convenient when a component design is constrained by space to have approximately the same solid volume for all material alternatives. Even when that is not the case, the engineer could provide relative estimates of the percentage differences in volume for the various materials. This is only possible when the mapping of inputs to outputs has the same linearly scalable relationship for all material alternatives. Prior research of the computational structure of LCA (Heijungs and Suh 2002) indicates that this should be the case, given several assumptions that will likely hold for this situation. This linear scaled relationship was confirmed by testing a large set of materials at various quantities of mass. There are numerous LCA-based impact assessment methods that can be used to determine environmental impacts from life cycle information. Although the 2003 version of environmental design of industrial products (EDIPs) was used to develop the methodology in this work, the MASSDOP method could also be applied to some of the other LCA impact assessment methods.

The additional advantage of using a data set expressed on a mass or volume unit basis for composites offers the means to expand the data set to include linear combinations of the impacts from the materials and their associated mass or volume fractions. Equation (1) shows the specific computation for the cell of each data point in the data set of a design space. An entry for a design alternative, i, in the design space is given by

$$\mathrm{D\,S}_{ij} = \left(\sum_{k=1}^{p} \mathrm{EIP}_{jl} \Lambda_{ik} \right)_i \mathrm{V\,E}_i, \tag{1}$$

where j is one of 14 different environmental parameters, k represents each of the materials in a composite, l is a material type that can be selected from among 72 different materials in a database, EIP_{jl} is the environmental impact parameter of a selected material l, Λ_{ik} is the volume

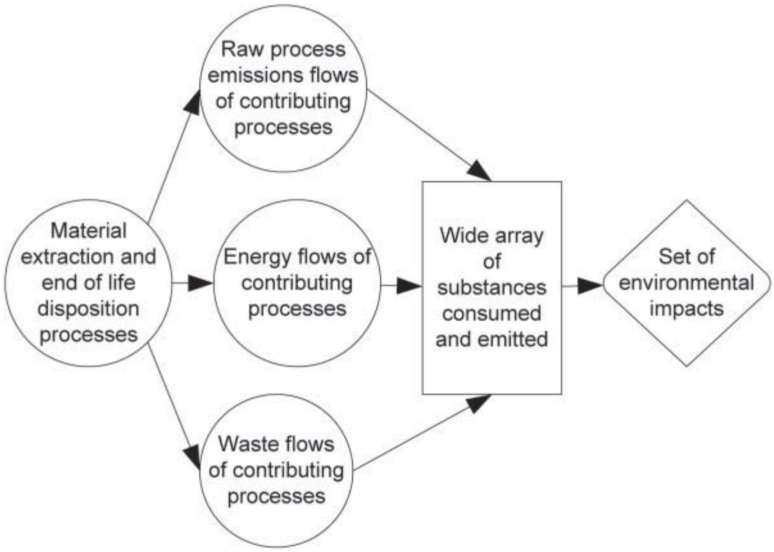

Figure 2. Mapping of the LCA process from the material selection perspective.

percentage of each material in a composite, and VE_i is the volume estimated fraction that a total composite is of a baseline.

The size of the design space can become virtually unlimited, given the wide array of potential materials. The information derived to compute the relative quantities of volume or mass is reused to compute factors of the life cycle cost attribute, recognising that the mass of a part is also a significant factor of both the material cost and the manufacturing cost. Later sections show how this data can be used to create surrogate models to identify optimal points where some potential unforeseen solutions could exist. Ecoinvent (Hischier et al. 2010) is available to use as an independent source[2] of information regarding material, energy, waste, and emissions flows. Figure 2 shows the schematics of how each material option has a set of numerous contributing processes and many corresponding substances emitted.

2.2. *Design attributes representation*

Multi-criteria decision-making (MCDM) methods were prescribed to evaluate design alternatives for traditional design (Gurnani, See, and Lewis 2003; Krishnamurty 2006; Thurston 2001, 2006). The life cycle impact assessment (LCIA) methods model environmental impacts into a form that can be represented as criteria in an MCDM model. The 2003 version of EDIP (Kietzmann 2000; Wenzel, Hauschild, and Alting 1997) for LCIA was deployed to develop the method presented here. Building on the authors' prior work to integrate LCA models into such a framework for engineering design (Eddy et al. 2013) and consistent with the findings identified in the recent works by Chandrasegaran et al. (2013), this paper introduces a method to represent the design space to select specific optimal sets of main components of a product for sustainability considerations. This approach provides the mathematical rigour of MCDM methods to the design of products for sustainability. For simplicity and brevity, this work represents the weighted sum of the fifteen main impact categories, or single score in Ecopoints [Pt] units, as a single environmental attribute.

A sustainable design should consider any effects on the people, planet, and profit (Bras 2005; Sarkar et al. 2009). Examination of these effects across a design space should include a data

Maximize Utility:

$$\boldsymbol{\Omega} = \{(\boldsymbol{f_1}(\overline{\boldsymbol{x}}), \ldots, \boldsymbol{f_p}(\overline{\boldsymbol{x}}))\}, \text{ where } \overline{\boldsymbol{x}} = (\boldsymbol{x_1}, \ldots, \boldsymbol{x_n})$$

Representative independent design variables:
$\boldsymbol{x_1}$ ... = Material types; $\boldsymbol{x_2}$ ... = Manufacturing processes employed; $\boldsymbol{x_3}$ = Mode of Distribution employed; $\boldsymbol{x_4}$ = Functional Priority; $\boldsymbol{x_5}$ = End of Life (EOL) Disposition; $\boldsymbol{x_6}$ ... = Part Volume (due to the geometry of the part)

Subject to:
$\boldsymbol{g_k}(\overline{\boldsymbol{x}}) \leq \mathbf{0} \quad \forall \mathbf{k}$ Compliance constraints

Select outcome from alternative set:

$$\boldsymbol{X} = \{\boldsymbol{X_1}, \boldsymbol{X_2}, \boldsymbol{X_3}, \ldots, \boldsymbol{X_m}\}$$

Representative attributes to minimize:
$\boldsymbol{f_1}(\overline{\boldsymbol{x}})$ = Total environmental impact = Pt
$\boldsymbol{f_2}(\overline{\boldsymbol{x}})$ = Cost = USD
$\boldsymbol{f_3}(\overline{\boldsymbol{x}})$ ... = Performance attribute(s) (problem specific)

Figure 3. Mathematical model for sustainable product design (Eddy et al. 2013).

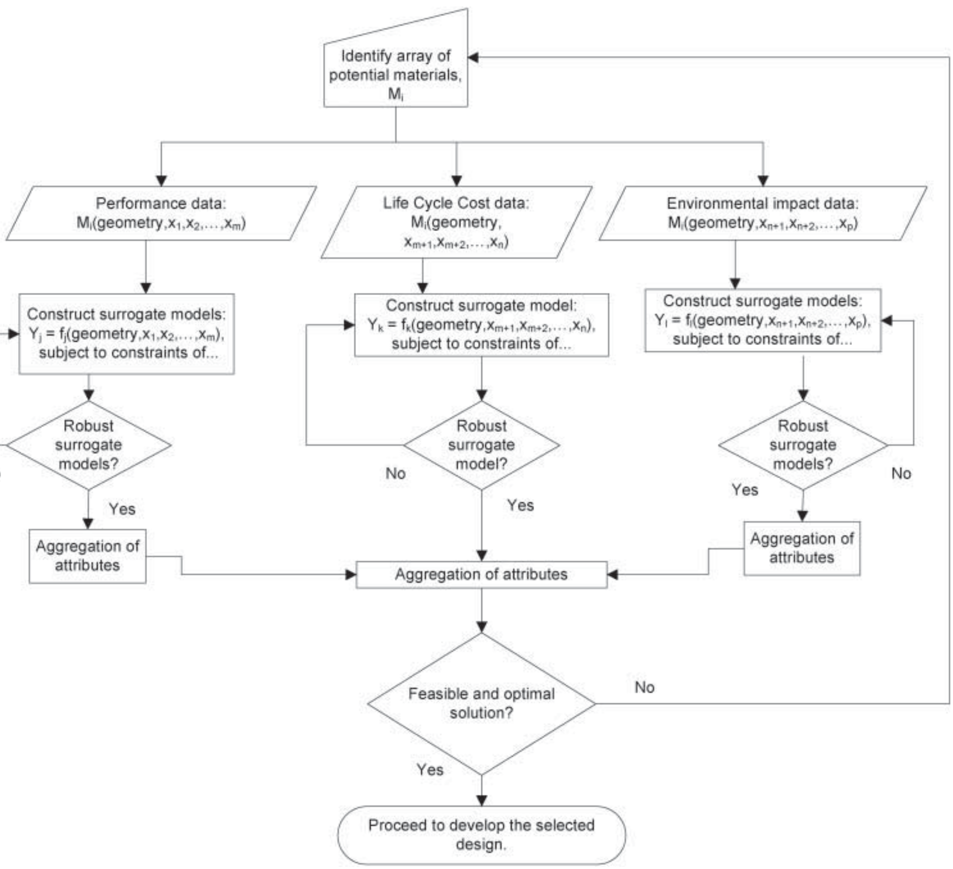

Figure 4. Methodology for a robust surrogate modelling approach for material selection in sustainable design of products (MASSDOP).

set from a diverse array of potential material options. Environmental attributes of a given material are a function of a set of environmental properties or factors in the form of processes that contribute during the significant life cycle stages as Figure 2 indicates. Traditional engineering design deploys established physical relationships between defined performance attributes and a set of mechanical properties of the materials. Similarly, life cycle cost attributes are mapped from a set of cost parameters associated with a given material. Since performance attributes can be defined in terms of those objectives that are most important to customers of the product or any other stakeholders, this formulation supports the triple bottom line objectives of sustainability to maximise the benefits to the people, planet, and profit.

The general mathematical multi-attribute model for sustainable optimisation problems formulated by this approach is shown in Figure 3. This model is based on the rationale and assumptions stated at the beginning of Section 2. It presumes that impacts from manufacturing and distribution are relatively negligible, and that main functions and form were determined at an earlier design stage by use of appropriate methods (Devanathan et al. 2010; Gilchrist et al. 2013; Srivastava and Shu 2013). The quintessential feature of the approach shown in Figure 3 is the ability to address design as a tradeoff between cost, performance, and total environmental impact. Since mathematical formulas to map design variables to their resulting attributes may not always be available, this paper advocates a surrogate modelling approach to obtain the needed mapping. As such, Figure 4 shows the mathematical construction of such a MAU formulation. Initially, the design space is represented by sets of data points associated with design alternatives. Linear correlations and regression models or other surrogate models are subsequently utilised to identify relationships between attributes and variables, as well as between different attributes. The selection of an optimal material in such a model is more complex in that the optimal solution is a certain distance away from the closest solution for which a material or set of materials exists. Here, Euclidean distance could be used to find the shortest distance in the vector space of a given alternative to the optimal. This computation would thus reveal the necessary changes to the independent variables towards identifying that new optimal material.

3. Mapping LCA factors to design attributes

This section covers the process by which environmental data sets can be formed to use for the surrogate model construction. The LCA of any given product, component, or unit mass of material is composed of several hundred different process contributions, which are composed of several hundred different substances of varying quantities emitted during the various processes. However, many of them contribute negligible quantities to environmental impacts. Thus, this work employs as a first step a tradeoff study on the model dimensionality and its accuracy.

3.1. *Tradeoff between model dimensionality and accuracy*

The question concerns how many of the variables with negligible magnitudes can be added into a single residual variable category. Significance of any residual term, such as error, could affect the accuracy and predictability of the model. However, if this residual term is reduced too much, the number of variables could be too numerous to include for model construction and optimisation. The following subsection describes a process to address this issue of dimensionality to derive an expression for the processes that contribute to the total Ecopoints [Pt] of environmental impacts caused by the extraction and end of life of a kilogram or cubic metre of a specific material.

3.2. *Design variables consolidation*

One approach to reducing dimensionality is to find an optimal cut off quantity under a certain percentage of the total. This cut off quantity could be based on keeping a percentage limit of

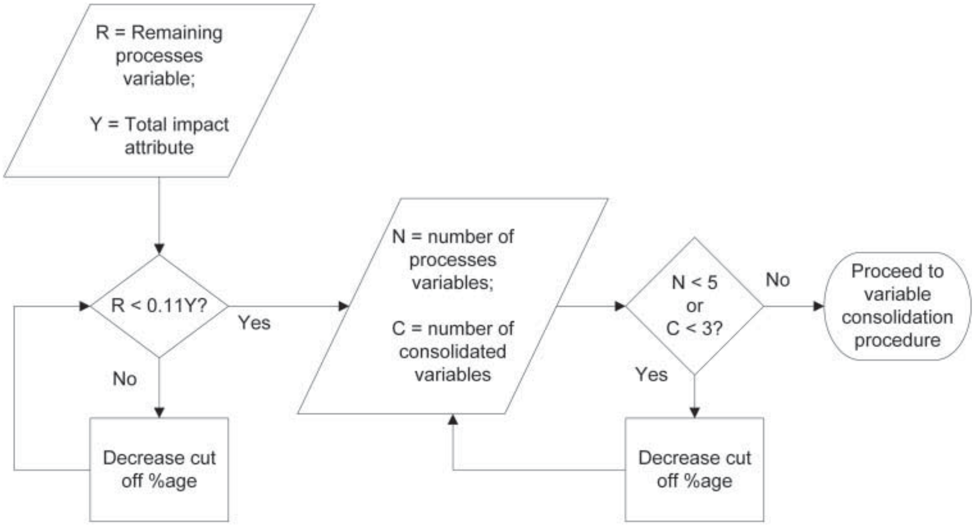

Figure 5. Process to include significant variables.

the total for the sum of the remaining processes. This work's preliminary study showed that a limit of 12% for the sum of the remaining processes, for 6 different materials in a test data set, kept the 'remaining processes' residual variable to a low level of significance in a surrogate model constructed by second-order polynomial regression. This process, shown in Figure 5, thus reduces the number of variables from several hundred down to anywhere from several to about 30 depending upon the category of environmental impact and the material that the LCA computation is generated for. Figure 5 also shows a subsequent check for $N < 5$ or $C < 3$ to ensure that the resulting relationship will have enough dimensions for a meaningful expression. A close look at the description of processes in all cases reveals that all processes can consolidate into one of the dozen categories listed in Table 1. These dozen variables are all one of three different types of flows in the life cycle processes: material production process flows, energy flows, and waste flows as shown in Figure 2. Thus, further reduction in the number of variables is achievable, but that would limit the amount of specific information. Some of the variables listed in Table 1 have lengthy descriptions in the first column, because the descriptions were broadened to include numerous more specific descriptions in the same row as part of the same variable as a result of this consolidation process. This consolidation to the dozen variables plus one residual variable, which all remain independent from each other, ensures a manageable dimensionality of this mapping of factors to the total environmental impact attribute.

The method to obtain a usable data point to map these processes to their associated environmental impact for a given material is now simplified to a three step procedure. First, each process is identified by the variable letter A through L of the category into which it fits. Second, all processes are sorted to align the variable letters together. Third, the processes of all values with the same variable letter are summed to compute the total value of that independent variable. Contributing processes and substances can both be expressed in weighted units of Ecopoints [Pt] for consistent comparisons. The value of the residual variable of remaining processes is labelled as R and was computed by the procedure described in the prior subsection. A final check for accuracy and scalability is done by adding the Pt values of variables A through L together with the value of R to check if the total sum is equal to that of the environmental impact's total value in Pt. This process was completed for all of the 72 most common raw materials found in the Ecoinvent database. These results are significant in two ways. First, the only known limitation of

Table 1. Descriptions of consolidated environmental variable categories.

Process	Variable	Project (Hischier et al. 2010; Goedkoop et al. 2008)	Unit
Total sum (output response) = sum of all input variables	*Y*		Pt
Major input variables identified categorically for materials	Independent variable		
Remaining processes	*R*		Pt
Final or raw material process /RER WITH US ELECTRICITY U	*A*	US-EI 2.2	Pt
Radioactive waste, in final repository for nuclear waste, or Uranium, enriched 3.8%, at USEC enrichment plant WITH US ELECTRICITY U	*B*	US-EI 2.2	Pt
Disposal, sulphidic tailings, off-site/GLO WITH US ELECTRICITY U	*C*	US-EI 2.2	Pt
Disposal, spoil from coal mining, in surface landfill/GLO WITH US ELECTRICITY U	*D*	US-EI 2.2	Pt
Process-specific burdens, residual or inert material, or sanitary, landfill (including slag compartment), or municipal waste incineration/CH WITH US ELECTRICITY U	*E*	US-EI 2.2	Pt
Disposal, sludge, remud, basic oxygen furnace wastes, average incineration residue, lead smelter slag, or hard coal ash, to residual material landfill WITH US ELECTRICITY U	*F*	US-EI 2.2	Pt
Disposal, spoil from lignite mining, in surface landfill/GLO WITH US ELECTRICITY U	*G*	US-EI 2.2	Pt
Hard coal (or Lignite), or heavy (or light) fuel oil, or natural gas (inc. sweetening), or pellets burned in power plant, gas turbine (compressor station), or industrial furnace/WITH US ELECTRICITY U	*H*	US-EI 2.2	Pt
Blasting/RER WITH US ELECTRICITY U	*I*	US-EI 2.2	Pt
Crude oil onshore or natural gas (inc. transported in pipeline, or sour gas in gas turbine), at production, or diesel burned in building machine or diesel-electric generating set, or transoceanic freight ship (or lorry operation)/WITH US ELECTRICITY U	*J*	US-EI 2.2	Pt
Disposal, hazardous waste, 0% water, to underground deposit or hazardous waste incineration WITH US ELECTRICITY U	*K*	US-EI 2.2	Pt
Disposal, municipal solid waste, 22.9% water, or inert material, 0% water, to sanitary or residual material landfill or municipal incineration WITH US ELECTRICITY U	*L*	US-EI 2.2	Pt

this approach so far is the availability of the LCI data for materials. Second, the resulting data set can be used as the seed data for any design problem by simple execution of Equation (1), which generates the data to construct a surrogate model for that specific design problem. Thus, the process described in this section must only be executed once and the results can then be applied to any product design problem. Since the surrogate models are constructed from these data sets with a limited residual percentage of the total impact and the surrogate models will be tested for robustness, the effectiveness of this procedure will be assessed in the following section.

4. Surrogate model construction

The first step in the construction of a surrogate model is to generate a set of data points. Such a data set was generated for the single score, or total environmental impact, of a diverse array of 72 different materials by using the method introduced in the above section. With such a significant number of data points, a portion of the data can be used to construct the surrogate model while the remaining data can be used to test the predictability of the model.

4.1. *Design space filling*

Data that represent material properties poses a unique challenge for the construction of a surrogate model. Such data have a specific and discrete location that is too inflexible for most sampling approaches. Conventional methods such as orthogonal arrays, Hammersley Sequence Sampling, Latin Hypercubes, and uniform designs (Sharif, Wang, and ElMekkawy 2008; Simpson, Poplinski et al. 2001) require strategic data locations that are uniform and balanced. Furthermore, some recent approaches that show promise for surrogate modelling with discrete variables have not yet been demonstrated for material selection (Peng et al. 2014; Simpson, Lin, and Chen 2001). The challenge is to find a way to approximate a viable space filling method to optimise model accuracy and robustness. The following subsections discuss the two-stage approach adopted in this work, based on an initial space filling sampling and subsequent sequential infilling sampling.

4.1.1. *Space filling sampling (SFS)*

Popular initial SFS methods include random sampling, stratified sampling, and Latin Hypercube. McKay, Beckman, and Conover (1979) showed that Latin Hypercube is typically at least as accurate for the examples they studied in comparison to both random sampling and stratified sampling. Thus, Latin Hypercube becomes the most obvious choice for this situation of non-flexible data locations for material alternatives. Even with multiple generations of the random locations within the cells, it is still very unlikely that locations can match exactly with data locations. Therefore, the resulting design is likely to be neither perfectly orthogonal nor perfectly rotatable. However, it is possible to find a Latin Hypercube design that minimises the Euclidean distances between the design points and the closest data points.

Several trials of executing this algorithm to find the minimum mean Euclidean distance among several runs from the data set of 72 materials are shown in Table 2. These results reveal that most of the designs generated with such material-related data call for design points to be filled by replicated data points. That is why it becomes necessary to repeat the search process for new data points. These trials revealed that the number of design points obtainable by this process is usually limited to not enough data to construct a surrogate model from. This is likely to be a real limitation in that there are no practical ways to increase the size of the cells to allow for more randomisation. Alternatively, the best surrogate models could be constructed by a two-stage process (Jin, Chen, and Sudjianto 2002; Kleijnen and Beers 2004; Montgomery 1984; Sacks et al. 1989) with the initial SFS followed by an SIS as detailed below.

4.1.2. *Sequential infilling sampling (SIS)*

Sequential infilling can improve the surrogate model accuracy and predictability because it uses information from the original sample. Many of the prescribed approaches for sequential infilling require data selection at predefined locations with minimal deviations (Booker et al. 1999; Hazelrigg 1999; Johnson, Moore, and Ylvisaker 1990) and are thus not applicable to this situation of

Table 2. Best index numbers of data identified by SFS.

Index numbers of materials identified				
Trial 1	Trial 2	Trial 3	Trial 4	Trial 5
30	6	2	40	40
2	1	1	6	1
22	22	2	1	40
40	40	30	30	2
44	6	30	44	40
30	40	30	6	40
40	2	40	40	30
6	40	22	30	2
40	40	22	44	40
40	40	1	40	6
22	2	6	44	40
6	30	6	2	27
30	6	40	44	44
40	30	6	2	30
44	40	30	40	1
1	44	40	44	1
2	30	39	6	30
2	44	30	30	40
6	44	2	40	2
40	30	40	30	16
6	1	1	6	30
42	22	44	6	30

material selection. The study conducted by Jin, Chen, and Sudjianto (2002) provides a comparison among various potential methods that could be evaluated for suitability for this situation. This study identifies some SIS methods that are most applicable only to evenly spaced designs with the Kriging predictive modelling method, such as Maximum Entropy, Mean Squared Error, and Integrated Mean Squared Error. The study also identifies other SIS methods that are not limited to the predictive models, such as Maximin Distance, and new proposed methods of Maximin Scaled Distance, and cross-validation.

This study by Jin, Chen, and Sudjianto (2002) compared these methods in six different examples. One of the examples is comparable to an environmental impact example in that it is non-linear with a dozen variables. Maximin Distance outperformed cross-validation in four of the six examples, and Maximin Distance outperformed Maximin Scaled Distance in the non-linear example with a dozen variables. Both Maximin Distance and cross-validation usually outperformed a one-stage approach without any SIS. The advantage of cross-validation is the lack of a need for new sample points, but that advantage is not applicable in this case where there usually are not enough sample points from the first stage. Maximin Scaled Distance allows for weights to be applied to all variables. The results indicate that any advantage may be mitigated for a higher dimension example. Therefore, the remainder of this paper focuses on the use of an SIS method of Maximin Distance. Maximin Distance prioritises those data points that have the furthest Euclidean distance away from points already in the sample set.

One important question concerns how much of the entire data set should be used to fill the sample set at this second stage and how much should remain to test the model. This paper addresses this critical issue by first examining the total single score environmental impacts in Ecopoints per cubic metre for all 72 different materials in the generated data set. The Latin Hypercube process presented in the prior subsection identified 14 data points to use for the original sample set. The chart in Table 3 shows the ordered list of the Maximin distances computed for the remaining data points. Although 22 more points would be needed to fill the sample set with half of the data, only the first several points in this example have significantly greater distances than other

Table 3. Maximin distances for SIS prioritisation.

Index numbers of materials in the remaining data set	Mean Euclidean distance of the data point to points in the original sample set
2	69.63
24	53.96
22	41.32
17	6.97
23	6.36
21	1.60
31	1.50
8	1.26
6	1.24
32	1.19
4	1.18
58	1.18
57	1.18
54	1.17
53	1.17
14	1.17
1	1.17
13	1.17
29	1.17
28	1.17
48	1.17
56	1.17
5	1.17
52	1.17
39	1.16

points. For example, when the size of the remaining sample set increased from the first nine data points to the top 22 data points, the average absolute error of the resulting model dropped from 8.7% (with four high leverage data points) to 3.8%. However, it is possible that a model with the smaller number of sample points could have better prediction accuracy of the points that are not included in the model. Criteria for testing the models are covered more in depth in Section 4.3.

4.2. *Response surface modelling*

Surrogate model construction techniques have advanced in recent years especially for computer experiments that sample with little or no error and use predefined and uniform data locations (Hazelrigg 1999; Kleijnen and Beers 2004; Shao 2007; Simpson et al. 2004). Here again, the discrete material selection process is a unique scenario. Kriging-based methods and second-order polynomial regressions offer two potential approaches to surrogate model building. While Kriging method has been shown to improve model accuracy in some cases over second-order polynomial regression (Jin, Chen, and Simpson 2001; Simpson et al. 1998), few studies have been conducted using Kriging in situations without uniform data locations.

Second-order polynomial regression should improve the model for optimisation purposes compared to the first-order linear model that was described in Section 3.2. The second-order model, unlike the flat plane of a first-order model, would emphasise the hill and valley optimal regions. However, since regression is a curve fitting approach, prior researchers have identified a potential issue with smoothing out the best regions of a curve (Hazelrigg 2003; Shao and Krishnamurty 2008). Therefore, this work compares the results of using both Kriging and second-order polynomial regression methods for response surface modelling. For the example described at the end of the last subsection with a sample size of 36 points, the R^2 adjusted was 100% for the second-order polynomial regression model compared to an R^2 adjusted of 28.64% for the Kriging model. For the same example with the sample size of 23 data points, the R^2 adjusted of the Kriging model improved to 98.40%, while the second-order polynomial regression model stayed at 100%. Results are likely to vary between data sets and for different examples. Therefore, each model should be tested and evaluated individually. The following subsection covers the model evaluation criteria.

4.3. *Model evaluation*

A designer would need to determine whether or not a constructed surrogate model is adequate to use to optimise for a given design situation. Research topics concern the accuracy of the model, the reliability of the model, and its robustness (Hazelrigg 2003; Shao 2007). Model accuracy is measured by how close sample points that are included in the model are to the model itself. Model reliability or predictability is measured by how close any points that are not included in the model are to the model itself. The model robustness takes into account the resolution between rank adjacent alternatives identified by the model and the effect of all variability due to the accuracy and reliability measures.

4.3.1. *Model accuracy*

From the original data set of 14 points identified by the Latin Hypercube method, the average absolute error measure is less than 0.1% when the second-order polynomial regression is used compared to 8.0% when Kriging method is used. Furthermore, a polynomial function is identified by the regression method to clearly define the surrogate model. Table 4 shows the results from the polynomial regression and accuracy measure for the complete set of 36 data points identified after the Maximin Distance SIS process. Both the mean and standard deviations, based on the assumption of normally distributed measures, are given for the average absolute error measures.

$$\mathrm{AAE} = \frac{1}{m}\sum_{i=1}^{m}\left|\frac{(y_i - \hat{y}_i)}{y_i}\right| = \bar{Y}. \tag{2}$$

Standard deviation is given by Equation (3).

$$S = \sqrt{\frac{\sum_{i=1}^{m}(y_i - y_{\mathrm{avg}})^2}{m-1}}. \tag{3}$$

4.3.2. *Model predictability*

Table 5 shows the actual and predicted values of the remaining 36 materials that are not included in the constructed model. Predicted values, labelled as YHAT, are calculated by substitution of all variable values at a data point into the polynomial function that defines the model. Results are shown here for the polynomial regression model as calculated by Equations (2) and (3) for the set of data that is not included in the sample set.

4.3.3. *Model robustness*

A model can be considered robust only if the variability that inherently exists in the approximate system does not prevent the selection of an acceptable design alternative. Thus, from a

Table 4. Model accuracy after the maximin distance sequential infilling sampling.

	After Infilling with Maximin distance:				
Residual	Absolute value of % error	Material	Y	Data point	% error
4.88E-04	0.0	Antimony	9665.366	2	0.0
− 1.23E-03	0.0	Molybdenite	7424.525	39	0.0
− 1.10E-03	0.0	Uranium natural	3809.048	22	0.0
1.44E-03	0.0	Copper	1562.633	31	0.0
4.36E-04	0.0	Lead	314.9437	18	0.0
− 1.63E-04	0.0	Silicon carbide	101.3786	44	0.0
6.49E-03	0.0	Nickel	2980.018	40	0.0
1.28E-02	0.0	Bronze	2641.319	4	0.0
4.96E-03	0.0	Iron nickel-chromium	1021.553	16	0.0
1.24E-03	0.0	AlMg3	142.6823	1	0.0
− 6.44E-03	0.0	Tin	734.3848	30	0.0
5.61E-03	0.0	Mischmetal	619.0798	42	0.0
− 2.24E-02	0.0	Brass	2077.479	33	0.0
1.54E-03	0.0	Magnesium-alloy AZ91	132.9016	43	0.0
2.50E-03	0.0	Aluminium	104.4364	29	0.0
5.74E-03	0.0	300 series stainless steel	172.0124	27	0.0
1.75E-03	0.0	Carbon	48.099	45	0.0
1.43E-02	0.0	Cobalt	376.6261	6	0.0
2.65E-02	0.0	Zinc	386.217	32	0.0
− 3.60E-02	0.0	Titanium zinc plate	441.8757	23	0.0
− 1.39E-02	0.0	Cast iron	88.04123	28	0.0
− 2.52E-02	0.0	Ferronickel	141.0945	11	0.0
2.08E-03	0.0	Charcoal	9.448632	46	0.0
− 3.04E-02	0.1	Epoxy resin	25.08595	9	− 0.1
− 4.06E-03	0.2	Brick	2.156056	3	− 0.2
1.60E-02	0.6	Limestone	2.568233	19	0.6
1.28E-02	1.2	Kiln dried lumber	1.091261	17	1.2
− 3.10E-02	1.2	HDPE granulate	2.604455	37	− 1.2
4.96E-02	2.1	Clay	2.386153	68	2.1
− 5.23E-02	2.8	Concrete block	1.898363	67	− 2.8
− 1.33E-01	3.0	Polybutadiene	4.415654	62	− 3.0
1.16E-01	9.3	Green veneer plywood	1.245942	38	9.3
− 2.62E-02	10.0	Asbestos (without use)	0.262908	71	− 10.0
2.67E-01	11.4	Scrap iron	2.355338	70	11.4
− 1.19E-01	15.7	Cold rolled sheet steel	0.756909	72	− 15.7
− 4.82E-02	80.6	Corrugated board	0.059796	7	− 80.6
Mean	3.8				
SD	13.7				

$Y = 0.05860287 + 1.237871{*}R + 1.056571{*}A + 1.008596{*}C + 0.7801412{*}D + 1.089715{*}E + 0.9841712{*}F + 0.6166319{*}G + 2.383661{*}H + 0.7763125{*}L + -0.004913406{*}R{*}R + -8.989214\text{E-}07{*}C{*}C + -0.007313005{*}E{*}E + 0.02540538{*}G{*}G + 0.01208991{*}I{*}I + 0.1854093{*}L{*}L + 0.007325138{*}R{*}D + -0.02496565{*}R{*}H + -0.05660541{*}R{*}L + 0.002324183{*}B{*}C + -0.000155864{*}C{*}G + 0.2967796{*}E{*}K + -0.4580382{*}E{*}L + 0.0291983{*}F{*}J.$

design perspective, a high fidelity model is not necessary if a surrogate model constructed from known data is sufficiently robust to select an alternative that is close enough to the optimal solution (Booker et al. 1999; Simpson et al. 2004). A designer would need to decide both on a tolerance for how close is acceptable and on the associated probability necessary for achieving that tolerance.

The statistical information computed in the two previous subsections enables the calculation of the robustness capability of a model. From a robustness perspective, one should consider the worst accuracy and the worst reliability at a given confidence level. The probability that both worst case limits could be reached at the same time would be the product of the probabilities for each individual occurrence. In other words, if a designer chose to remain within one standard deviation of both the mean accuracy and the mean reliability, there would be a 15.87% chance of either limit being reached or a 2.52% chance of both limits being reached at the same time.

Table 5. Model predictability and robustness test.

YHAT from model	Residual	Absolute value of % error	Material	Y	Data point	% error
21.0253	3.19216	13.2	Ceramics	24.21751	5	13.2
1.64257	0.09908	5.7	Dry veneer plywood	1.741654	8	5.7
6.36742	– 0.21993	3.6	EPS	6.147493	10	–3.6
7.35121	0.25672	3.4	Glass	7.607927	12	3.4
2.52608	– 0.32039	14.5	Graphite	2.205688	13	–14.5
6.80192	– 0.39608	6.2	HDPE	6.405836	14	–6.2
8.27397	– 2.14558	35.0	HIPS	6.128396	15	–35.0
128.101	0.95016	0.7	Magnesium	129.0515	20	0.7
26.034	1.29545	4.7	Zinc Oxide	27.32944	21	4.7
10.3047	2.77498	21.2	Synthetic rubber	13.07966	24	21.2
34.181	– 0.25573	0.8	Silicone	33.92523	25	–0.8
80.3126	– 2.34415	3.0	Low alloy steel	77.96843	26	–3.0
13.8747	– 1.60897	13.1	Nylon 6	12.26568	34	–13.1
6.71235	0.11133	1.6	Oriented strand board	6.823673	35	1.6
8.29699	– 0.60612	7.9	PVC	7.690876	36	–7.9
60.5247	– 0.33096	0.5	Lithium	60.19372	41	–0.5
38.6013	– 1.95874	5.3	Polyester resin glass fibre	36.64257	47	–5.3
19.7913	5.24172	20.9	MG-silicone	25.03306	48	20.9
17.3331	– 2.2138	14.6	Polycarbonate	15.11933	49	–14.6
48.324	– 2.99063	6.6	Ferrochromium	45.33334	50	–6.6
13.7786	– 0.91003	7.1	Nylon 66	12.8686	51	–7.1
13.6577	– 0.85044	6.6	Nylon 6 glass filled	12.80728	52	–6.6
4.51	– 0.28627	6.8	Polyurethane rigid foam	4.223724	53	–6.8
21.9634	0.37598	1.7	Glass fibre	22.33937	54	1.7
12.5796	– 0.94939	8.2	Nylon 66 glass filled	11.63016	55	–8.2
6.56019	– 0.08904	1.4	Polypropylene	6.471152	56	–1.4
6.52119	– 0.58117	9.8	Low Density Polyethylene	5.940023	57	–9.8
24.3	2.69254	10.0	Ferrite	26.99254	58	10.0
36.6571	2.36725	6.1	Ferromanganese	39.02432	59	6.1
24.7372	0.42559	1.7	Magnetite	25.16274	60	1.7
3.99239	– 0.08468	2.2	Polystyrene GPPS	3.90771	61	–2.2
30.5089	4.90078	13.8	Pig iron	35.40968	63	13.8
39.7899	0.56287	1.4	Cadmium	40.35274	64	1.4
2.62116	0.39422	13.1	Laminated veneer lumber	3.015381	65	13.1
1.75393	0.16692	8.7	Plywood	1.920851	66	8.7
2.02638	– 0.19374	10.6	Bauxite	1.832641	69	–10.6
	Mean	8.1				
	SD	7.2				
			Model accuracy:	Mean	3.8%	
				SD	13.7%	
			Model reliability:	Mean	8.1%	
				SD	7.2%	

97% confidence that 32.8% is the most that any value will deviate from the model.
Since one material to the next differs by 14.9% on average, there is 97% confidence that a material selected from this model will be within 2.2 materials of the actual optimum.

For the example shown in Tables 4 and 5, the sum of the means and standard deviations of the accuracy and reliability error values is a total of 32.8% error. Therefore, there is a 97.48% confidence level that the error will be less than 32.8% when this model is used based on the data used in this test. Next, a designer would need to calculate the average resolution between alternatives. Here, one could simply rank order the 72 different alternatives and calculate the average difference in the values between each of the adjacent pairs of alternatives. Thus, for a set of alternatives, X, resolution is given by Equation (4).

$$\text{Resolution}_{\text{avg}} = \frac{x_{\max} - x_{\min}}{(n-1)x_{\text{avg}}}. \tag{4}$$

The expected number of alternatives from best is given probabilistically with 97% confidence on average by Equation (5).

$$\#\text{ of alternatives displaced}_{\text{avg}} = \frac{\bar{Y}_{\text{in model}} + S_{\text{in model}} + \bar{Y}_{\text{not in model}} + S_{\text{not in model}}}{\text{Resolution}_{\text{avg}}}. \tag{5}$$

For the example shown in Tables 4 and 5, the resolution is 14.9%. Therefore, a designer could be 97.48% confident of selecting an alternative inferior to the best by no more than 2.2 places on average as determined from Equation (5). In other words, it is very likely that an alternative in the top three of the 72 material alternatives would be selected by using this model. If that expectation is acceptable to the designer, this surrogate model can be considered sufficiently robust. However, if the results are not satisfactory, the designer may need to increase the total number of data points or improve either the initial sampling procedure or the subsequent SIS or the surrogate model building process.

5. Optimal design selection using MAU model

Equation (1) provided a systematic approach to problem formulation by converting standard data into problem-specific data sets. Here, the generation of a data set for the environmental attribute is computed directly from Equation (1). Masses of the components can be computed by simply multiplying the part volumes and the material mass densities. The masses are also variables that the life cycle cost attribute depends upon. The remaining cost data and data sets for performance attributes are problem specific, and should be determined by a designer for a specific case.

5.1. *Single attribute optimisation*

Each attribute is a function of variables upon which a different attribute could also depend. Tradeoffs could exist where a change in that variable could cause one attribute's utility to increase while another decreases (Keeney and Raiffa 1993). Thus, it is important to optimise each attribute's utility model individually to observe the effect of all known and potential dependent variables. A utility function can introduce some additional non-linear effects beyond any that exist in a function of the attribute values as examples in a prior work indicated (Keeney and Raiffa 1993). All single attribute models can then be compared side by side at the same optimal data point locations to construct or visualise the Pareto optimal frontier (Keeney and Raiffa 1993) for the next step covered in the following subsection.

5.2. *Optimisation of multiple attributes*

Preference modelling methods can identify a specific optimal point on a Pareto optimal curve. The MAU function is a composite linear combination of the single attribute values and their preference weights (Hazelrigg 2012). Therefore, the optimal solution predicted by a surrogate model of the MAU function should be close to the composite linear combination of the values predicted by the SAU surrogate models. This is an important check. The goal is to find the maximum MAU value in the feasible region. Prior approaches were able to improve optimisation with surrogate models by clustering to find more accurate points in the optimal regions of interest (Shao and Krishnamurty 2008). However, the optimal solution may not be located at a data point where a known material exists. Alternatively, the Euclidean distance between the optimal point or points and the known data points offers an excellent metric to reveal not only the closest known solution, but also, a change in certain data values that could result in a better solution than was originally realised.

5.3. *Feasible region to comply with regulations*

Many traditional design optimisation problem formulations include constraints that define the feasible and infeasible regions of a design space. The environmental considerations of design for sustainability can introduce additional constraints to a problem in the form of standards or regulations that require compliance. Previous work demonstrates a way to reveal such information transparently for integration at the early design stages (Eddy et al. 2014). A key issue concerns the degree to which such information can be represented as constraints in an optimisation formulation. That would depend upon the mathematical alignment of a given standard with an LCA computational structure. Instead, standards can be best included as mathematical limits in a constrained optimisation problem when it is possible and practical to do so. Otherwise, the best approach may be to red flag any data points or design regions of concern for application of a penalty to the MAU value where any constraints are not met.

5.4. *Sources of uncertainty*

Section 4 provided a prescriptive method to account for uncertainty in constructed surrogate models and the associated confidence for selection of materials. A designer should realise that there are also other sources of uncertainty. For one, parametric uncertainty can be significant in both the assessment of environmental impacts and costs over a product's life cycle, as was pointed out in a prior study (Eddy et al. 2013). Previous works prescribed methods to represent such uncertainties in utility formulations by deployment of expected utility functions over the interval of each attribute (Gurnani, See, and Lewis 2003; Jin, Du, and Chen 2003). For brevity, the execution of such established methods is not replicated in this paper, which only represents the mean values of parameters in all formulations.

Uncertainty also results from the simplifying assumptions made in Sections 2 and 3. In Section 2, the focus was to find the most significant life cycle stages of a product. Relative to material selection, impacts from manufacturing and distribution are likely to be negligible for many products. Also, it is presumed that product use impacts are predetermined by a separate process in a previous design stage. However, that will not necessarily be the case for all products. Since it is not feasible or practical to analyse the validity of these assumptions for every potential type of product in the scope of this paper, it is recommended that designers assess such effects on a case-by-case basis.

The process described in Section 3 involves a tradeoff between dimensionality and accuracy, which generates a residual variable R for remaining processes. This is an error term that was minimised by that process. Since this variable R appears as a parameter in the optimisation formulation, the designer can assess the significance, confidence, and risk posed by it in each individual case. Given these stated assumptions, the next section demonstrates the application of the entire methodology in a practical example design problem.

6. Case study: sustainable design of an automobile disc brake

This case study is an application of the procedures exactly as they were described in detail in the prior sections. Common performance objectives for the design of a set of rotor and caliper pads include minimisation of the vehicle stopping distance, minimisation of mass needed to allow for wear and also ensure acceptable life of the components, and adequate dissipation of heat as the components are near the end their life. For this example, it was assumed that the desired life is five years and that the temperature in the rotor and pads should never exceed 77°C. Results for specific design alternatives were calculated by using the conventional engineering formulations (Shigley and Mischke 1986). Some information was obtained to estimate the specific values of rotor material property parameters (Maleque, Dyuti, and Rahman 2010). For illustrative purposes, the best reasonable values were estimated of material property values. This example provides a useful illustration of a practical design situation that involves consideration of a variety of pure and composite materials. The example further demonstrates the simultaneous consideration of performance, environmental, and economic objectives.

6.1. *Problem formulation*

To simplify the illustration, a single performance objective of minimising vehicle stopping distance was used. That objective depends upon the coefficient of friction between the rotor and pad materials based on assumptions of reasonable operating conditions. From there, adequate heat dissipation was treated as an additional constraint. The initial minimum solid volume of the rotor and pads was computed for each design alternative at the given constraint values. For this example, the solid volume of the pad was proportional to the pads' initial thickness due to constant area, and the rotor's solid volume was represented as a function of the initial rotor thickness and the solid volume percentage, since rotors are usually casted to a hollowed shape to add a convection cooling feature. LCA and life cycle costing formulations indicate that minimisation of mass for a given material would directly help to optimise both of these objectives.

Table 6 shows rotor alternatives identified by prior work (Maleque, Dyuti, and Rahman 2010) along with pad alternatives found from general searches in prior work (Eddy et al. 2014). Six different possible rotor materials are labelled 'A' through 'F', and eleven different potential pad materials are labelled '1' through '11'. Every possible material combination is labelled by the letter of the rotor followed by the number of the pads' material. Material combinations flagged by a red, or lighter, font in Table 6 are a concern based on regulations of copper content in two states ('Limiting Copper in Brake Pads' 2013; 'The Better Brakes Law' 2013).

Some of the combinations were found to be infeasible for the given temperature limit and heat dissipation and life requirements. This resulted in a total of forty-six alternatives of material combinations in the original design set (Eddy et al. 2014). From the derived information,

Table 6. Matrix of known design alternatives (Maleque, Dyuti, and Rahman 2010).

	Rotor materials					
	GCI (grey cast iron)	Ti-alloy (Ti-6Al-4V)	7.5% wt WC and 7.5% wt TiC reinforced Ti-composite (TMC)	20% SiC reinforced Al-composite (AMC 1)	20% SiC reinforced Al-Cu alloy (AMC 2)	Ceramic composite
Pad materials						
Semi-metallic	A1	B1	C1	D1	**E1**	F1
Ceramic compounds	A2	B2	C2	D2	**E2**	F2
Mineral (synthetic silicate) fibres	A3	B3	C3	D3	**E3**	F3
Aramid Nomex fibres	A4	B4	C4	D4	**E4**	F4
Kevlar fibres	A5	B5	C5	D5	**E5**	F5
Twaron fibres	A6	B6	C6	D6	**E6**	F6
PAN	A7	B7	C7	D7	**E7**	F7
Chopped glass	A8	B8	C8	D8	**E8**	F8
Steel	A9	B9	C9	D9	**E9**	F9
Copper fibres	**A10**	**B10**	**C10**	**D10**	**E10**	**F10**
Other plastics	A11	B11	C11	D11	**E11**	F11

Note: The bold values are concern of greater than 0.5% copper content.

estimates were made for the percentage volume composition of each composite material. This information allowed generation of the entire data set for the single score environmental impact by applying Equation (1). Volume data were converted to mass for each alternative to generate the data set for the life cycle cost attribute. Additional data of moulded pads cost per unit mass and rotor material cost per unit mass were also estimated for each alternative to complete the life cycle cost data set.

6.2. *Surrogate model construction and testing*

If the goal of this design project were simply to select the best known design alternative, then a surrogate model would not need to be constructed. The design alternative with the greatest MAU value for a given stated preference among the attributes would be the optimal design concept to proceed with for this given set of alternatives. However, if a designer needs to view a design space to find whether or not any potentially more optimal solutions exist, surrogate models of each individual attribute and the composite MAU response can facilitate such an investigation. Traditionally, single attribute response variables are labelled as 'u' followed by an attribute subscript number and the MAU variable is labelled as 'U'. For this example, it was assumed that a designer's preference is represented by the vector of $\{p = 0.214, c = 0.429, \mathrm{ei} = 0.357\}$ representing performance (p), cost (c), and environmental impact (ei).

Table 7 shows the surrogate model function constructed for this specific design example by applying the methods introduced in Section 4. Here, it was evident that the Latin Hypercube space filling followed by the Maximin Distance sequential infilling resulted in a model accuracy, which was explained in Section 4.3.1, with less than 0.1% absolute error. Table 7 illustrates the test for model predictability by comparison of actual responses to those predicted by the model. These results show a significant difference between the model reliability predicted by all data points and that predicted when only those points in the neighbourhood of optimal response values ($U > 0.5$) are included in the absolute percent error computation. If a designer can assume that data points with small MAU values would not be selected as optimal, the expected model robustness would improve. The 97% confidence level would then improve on average from an alternative selected in the top seven to the top two of the forty-six alternatives in this design set. The following subsection illustrates a methodical approach to mitigate any risk involved in making such an assumption.

6.3. *Search for the optimal solution in a design space*

In the prior subsection, the expected differences between actual and predicted MAU values in an alternative set were investigated. Figure 6 shows the actual utility values of each single attribute and of the composite MAU plotted by the bottom four curves in the legend. Section 5 described a method that could be used to find the global optimal point(s) in the design space by using an acceptable surrogate model. In this example, the lack of any tradeoff among the attributes, evidenced by Figure 6, poses some challenges with finding a single optimum point. In this case, the GA was used to search globally for potential optimal solutions. Several hundred of the final iterations identified predicted MAU values over 0.95.

As Section 5.2 points out, the optimal point(s) may not be located near where an actual material exists. For a case such as this one, it is recommended to find optimal points with a Euclidean distance as close to a known alternative, given in Table 6, as possible. In Figure 6, the corresponding alternatives are shown on the horizontal axis from left to right ordered by shortest Euclidean distance to a predicted target optimal point. One could expect a potential accuracy issue with predicted optimal points on the outskirts of a design space away from the limited design set

Table 7. Results from testing the constructed surrogate model for multiple attributes (MAU).

Polynomial regression had an R^2(adj.) = 100.00%

MAU = 2.531906 + − 1.087753*inverse of coefficient of friction + − 0.006607899*B + − 0.006222348*I + 0.1701313*inverse of coefficient of friction*inverse of coefficient of friction + − 0.0004935422*rotor raw material cost only in USD/kg*rotor raw material cost only in USD/kg + − 0.00187399*disc mass in kg*J + − 0.0003781217*pads cost in USD/kg includes moulding*F + 0.002449867*rotor raw material cost only in USD/kg*H + − 0.003641434*rotor raw material cost only in USD/kg*I + − 8.202102E-06*C*D + − 0.001039736*I*K

For the data points not included in the PR model:

YHAT	Residual	Absolute value of % error	Alternative #	Y	Data point	% error
0.927	− 6.09E-03	0.7	A9	0.933	9	− 0.7
0.820	− 1.41E-02	1.7	A3	0.834	3	− 1.7
0.860	3.35E-02	4.1	F9	0.826	45	4.1
0.844	1.99E-02	2.4	A10	0.824	10	2.4
0.811	− 7.37E-03	0.9	A2	0.818	2	− 0.9
0.781	2.12E-02	2.8	F1	0.760	44	2.8
0.756	− 2.51E-03	0.3	E8	0.759	40	− 0.3
0.776	2.01E-02	2.7	F10	0.756	46	2.7
0.724	− 5.56E-03	0.8	E11	0.730	43	− 0.8
0.711	− 1.25E-03	0.2	E5	0.712	37	− 0.2
0.699	− 4.60E-03	0.7	D11	0.704	32	− 0.7
0.683	− 1.15E-02	1.7	D3	0.694	24	− 1.7
0.668	4.62E-03	0.7	D2	0.663	23	0.7
0.599	− 2.03E-02	3.3	E9	0.619	41	− 3.3
0.615	8.63E-04	0.1	E7	0.614	39	0.1
0.597	− 6.68E-04	0.1	D7	0.598	28	− 0.1
0.233	4.56E-02	24.3	C9	0.187	19	24.3
0.217	3.45E-02	18.9	C8	0.183	18	18.9
0.202	2.52E-02	14.3	C4	0.177	14	14.3
0.213	4.06E-02	23.6	C1	0.172	12	23.6
0.139	5.17E-03	3.9	C3	0.134	13	3.9
0.181	5.43E-02	42.9	C11	0.127	21	42.9
0.045	6.65E-03	17.3	C10	0.038	20	17.3
	Mean	7.3				
	SD	11.1				
If low Y values are excluded						
	Mean	1.4				
	SD	1.2				
	Resolution	3.3				

Throughout this design set, if low Y values are excluded, there is a 97% confidence on average of being within 0.82 alternatives of the best value.

of discrete material-related data locations that were available to construct the surrogate model. Thus, Figure 6 shows a significant difference between the actual and predicted MAU values of the target points. The mean difference is 27% with an 11.5% standard deviation, which is significantly higher than that found in the prior subsection. However, Figure 6 shows that alternative A9 has a MAU value that exceeds any of the actual target points.

It is notable that this is the same concept that would have been selected without a surrogate model. This suggests that surrogate modelling could be as effective in some cases as full computations of the MAU values of each alternative without the efforts of the full computations. Furthermore, it would be difficult to confirm the superiority to other potential solutions without any surrogate model. If hypothetically the results showed that a different potential better solution did exist, a designer could easily compare the values of all the design variables between the target point and the closest alternative in the design set. This would show a designer how a search for materials with slightly different specific properties could improve the design. Furthermore, this problem was solved both before (Eddy et al. 2014) and after this MASSDOP

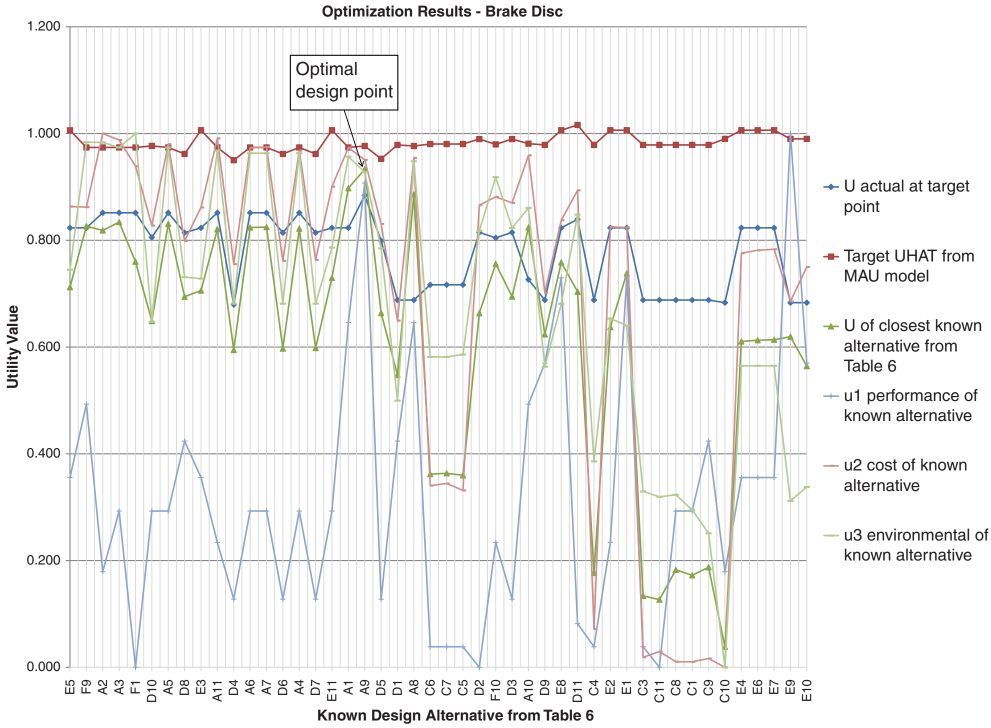

Figure 6. Results from optimisation of a brake disc design.

method was developed. In addition to a view of the design space not previously realised, the design process with MASSDOP took only about 25% of the time to execute compared to a prior method of manually modelling a complete LCA for every design alternative, which took about 20 hours longer. The MASSDOP method as deployed in this example could be extendable to other practical engineering design problems.

To complete the assessment of such a case study, a designer should consider the impact of all sources of uncertainty based on the assumptions that were summarised in Section 5.4. For this case, based on the modelling uncertainty alone, as shown in Table 7, there is 97% confidence on average of selecting one of the top two material combinations. As noted, the modelling uncertainty could increase in optimal regions far away from any know data points. The residual variable R, which was derived in Section 3, does not appear in the regression formula generated in Table 7. Thus, that variable R is not significant in the surrogate model of this case study example.

There are other sources of uncertainty. This study and the prior study to which it was compared used only the mean values of all parameters. If a decision-maker was most concerned about prevention of the worst possible environmental impacts and the worst possible cost based on significant parametric uncertainty, than a different material combination may need to be selected. There were also some simplifying assumptions about the life cycle. In this case, the effects of impacts at the product use stage are negligible, because the differences in wheel inertia that could affect vehicle millage are very small. Similarly, impacts from the distribution stage are likely to be small due to the size of these parts. It does appear likely for this case that the assumption that impacts from manufacturing are negligible is reasonable for the sake of selecting the optimal bill of materials, as suggested back in Figure 1, because the same best alternative was selected from both the use of this method and from construction of a full LCA for each alternative in the original set.

7. Discussion

This work addressed several main objectives. First, the investigation concerned the efficient and effective integration of credible LCA computations into the early stages of a design process along with traditional design objectives to represent all significant and pertinent life cycle stages. Second, the work addressed the challenge of the construction of usable surrogate models to identify optimal solutions that consider multiple objectives that include LCA across a design space beyond a mere set of known design alternatives. Third, the construction of usable surrogate models for material selection with such sustainability considerations involves the additional challenge of using data points in the design space that are not in desirable locations for traditional design SFS techniques. Fourth, it was necessary to demonstrate the effective and efficient deployment of the MASSDOP method in a practical and realistic design example. This section discusses the results of this work in the context of these established objectives.

Traditional use of LCA methods enables an accurate evaluation of the environmental impacts of a specific product design. However, such accurate methods are difficult to use efficiently to compare design concepts during early design stages. Approximate methods have been prescribed for the purposes of efficient concept selection in traditional product design. This work focused on significant factors to enable efficient identification of concepts. It is also important to account for all objectives over an entire product life cycle. Since other works introduced methods to account for the life cycle stage of product use (Devanathan et al. 2010; Gilchrist et al. 2013; Srivastava and Shu 2013), some design situations may ideally involve the use of a combination of the other works with this one. Thus, this work focused on the accounting of all other stages of significance with more accurate computations of the impacts from LCA. Investigation indicated that material selection is often the most significant factor beyond the basic form and function associated with a product's use. Since environmental impacts are output responses and material selected is a single variable with a set of parameters associated with each alternative, the challenge involved identification of a usable set of significant environmental parameters from the high number of parameters associated with each environmental impact. Section 2 covered the rationale for a foundation of the methodical approach described in Section 3 to address this issue.

Further efficiency can be gained from the ability to generate a data set by the formulation given by Equation (1) in Section 2.1. This approach addresses another important issue about the potential for human–computer interaction, which could be vital to the adoption of any method or tool at the early design stages. Such a tool for this formulation can be completely interactive with the user. User prompts could include: how many material combinations to consider, how many materials in each specific alternative, percent composition of each material selected, and the volume percentage of each alternative as a percentage of a baseline volume. A program can automatically generate the entire data set from the information entered. Another program can be used to construct surrogate models from the data, and another program can perform optimisation after the models are constructed and tested. With additional coding, all such programs could be integrated together and include appropriate user interfaces to achieve automation or semi-automation of this method execution. Such automation could help justify the effort involved with using the MASSDOP method at the early design stage when it would be most influential in the selection of the optimal bill of material.

Section 3 prescribed a technique to map input parameters to output responses that is essential for surrogate model construction as described in Section 4. The use of surrogate modelling can be ideal to efficiently streamline the complex computational structure of both LCA and traditional physics-based formulations of predictive product performance. Section 3 also identified two important topic areas in need of further research. Both the impacts predicted by LCA and performance objectives can involve multiple attributes that require some aggregation. A key further research topic involves various approaches to group the attributes and to model the preferences among the attributes in the groups. Here, tradeoffs can exist both among performance or environmental objectives and also between the overall objectives of minimising cost and environmental impact and maximising performance objectives. Although the case study presented here does not happen to exhibit such tradeoffs, it does provide a useful demonstration of how this MASSDOP method can be deployed in a practical engineering design problem. Other future examples could exhibit tradeoffs between objectives such as environmental impact and the deflection or stability of a component.

One of the key contributions of this work was the development of a method to construct surrogate models for this particular type of problem that can also consider all objectives in the decision model efficiently and effectively for concept selection. Section 4 described this method in depth. This development included the investigation of possible SFS and SIS two-stage approaches to adapt and deploy in ways that address the unique challenges of material selection specifically for sustainable product design. Useful examples were presented in both Sections 4 and 6, where an actual case study of a product design was demonstrated. Here, the issues of model accuracy, reliability, and robustness were addressed given any limitations posed by the dimensionality and sample size of a data set. Given the promising results, future work could look at the potential to further improve both robustness and design efficiency by deployment of more recent surrogate modelling approaches, such as a technique identified in Section 1 (Swiler et al. 2014), to this domain of sustainable product design. Section 5 explained how usable models of a design space can identify optimal solutions that consider all the objectives. With this approach, better solutions may possibly be identified efficiently beyond simply selecting the best alternative from among a set of the previously known alternatives as the case study demonstrated in Section 6. Furthermore, in this example, the same results were obtained both with and without the surrogate model, which suggests that this MASSDOP approach could significantly reduce computational efforts without sacrifice of effective concept selection in some cases.

8. Summary

This work focused on material selection for the most significant effect on sustainability objectives in the early design of product components. Challenges for efficient and robust surrogate model construction include the inflexible discrete locations of material-related data points and the dimensionality of the data. To address these challenges, a technique was developed to both streamline the LCA model construction for viable material alternatives and simplify model dimensionality by the consolidation of factors. This enabled the construction of robust surrogate models of the environmental objectives in a rigorous representation with other traditional design objectives. The feasible approximation approach for model sampling addressed the challenges posed by the associated rigid data locations of these material-related parameters. Robust results can be achieved by use of the presented adapted Latin Hypercube approach at the first of two sampling stages. Such an approach enables optimal concept identification within a design space beyond the original data set of known design alternatives. Two examples illustrate the potential for reasonable robustness at the early design stages.

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Notes

1. This paper is an extension of two different prior versions that appear in Eddy (2014). Sustainability-based product design in a decision support semantic framework. http://scholarworks.umass.edu/dissertations_2/76, and also portions are reprinted by permission of the publisher American Society of Mechanical Engineers (ASME) of the version Eddy, Krishnamurty, Grosse, Wileden, and Lewis (2014, August). A robust surrogate modelling approach for material selection in sustainable design of products.
2. http://www.ecoinvent.org/database/.

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