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Sustainability-Based Product Design in a Decision Support Semantic Framework

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**SUSTAINABILITY-BASED PRODUCT DESIGN IN A DECISION SUPPORT
SEMANTIC FRAMEWORK**

A Dissertation Presented

by

DOUGLAS C. EDDY

Submitted to the Graduate School of the
University of Massachusetts Amherst in partial fulfillment
of the requirements for the degree of

DOCTOR OF PHILOSOPHY

May 2014

Mechanical Engineering

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**SUSTAINABILITY-BASED PRODUCT DESIGN IN A DECISION SUPPORT
SEMANTIC FRAMEWORK**

A Dissertation Presented

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DEDICATION

To all engineers who seek to consider the impacts of their designs.

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ABSTRACT

SUSTAINABILITY-BASED PRODUCT DESIGN IN A DECISION SUPPORT SEMANTIC FRAMEWORK

MAY 2014

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The design of products for sustainability involves holistic consideration of a complex diversity of objectives and requirements over a product's life cycle related to the environment, economics, and the stakeholders in society. These objectives may only be considered effectively when they are represented transparently to design participants early in a design process. Life Cycle Assessment (LCA) provides a credible prescription to account for environmental impacts. However, LCA methods are time consuming to use and are intended to assess the impacts of a completely defined design. Thus, more capable methods are needed to efficiently identify more sustainable design concepts.

To this end, this work introduces a fundamental approach to formulate models for normative decision analysis to accurately account for these multiple objectives. Salient features of this novel approach include the direct accounting of the LCA formulations via mathematical relationships and their integration with derived expressions for compatible life cycle cost models, as well as a methodical approach to account for significant sources of uncertainty. Here, a semantic ontological framework integrates the information associated with decision criteria with that of the standards and regulations applicable to a design situation. Since this framework shares the context and meaning of this information and design rationale across domains of knowledge transparently among design participants, this approach can influence a design toward sustainability considerations while the design complies with regulations and standards.

Hypothetical equivalents and inequivalents method is represented and deployed to consistently model a designer's preferences among the criteria.

Material selection is a very significant factor for the optimal concept selection of a product's components. A new method is detailed to estimate the impacts of material alternatives across an entire design space. Here, a new surrogate model construction technique, which is much more efficient than the construction of complete LCA models, can prune the design space with adequate robustness for near optimal concept selection. This new technique introduces a feasible approximation of a Latin Hypercube design at the first of two sampling stages to overcome the issues with sampling from discrete data sets of material property variables.

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CHAPTER 1

BACKGROUND AND MOTIVATION

Product lifecycles account for a significant proportion of the total consumption of the planet's constrained environmental, non-renewable, and economic resources. While these product lifecycles are becoming shorter, the diversity of products is becoming larger. Thus, significant improvements in the optimal design of products for sustainability will reduce the load on the environment, economy, and society. The design of products for sustainability is a complex issue that involves several different topic areas. . It has been shown that significant advances toward sustainable product design can be gained by appropriate improvements in lifecycle design processes [1]. Existing approaches to supporting sustainable product design tend to be focused on the later stages of product development, focusing on assessment of environmental impact costs after a design is selected, but not to include the early stages of design decision making. Support for more sustainable decisions during the conceptual design stages can lead to numerous advantages for enterprises. Prior research by Bras [2] finds that enterprises that focus on the triple bottom line objectives of the environment and society in addition to the economic dimensions realize additional value added returns. By focusing on triple bottom line objectives during product design, the people, planet, and profits are likely to be preserved for a longer period of time and a new paradigm for the competitive design of products is likely to be established.

A recent NIST (National Institute of Standards and Technology) workshop on sustainable manufacturing [3] addresses the industry needs and identifies the needs for better decision support tools, strong mathematical models to support the decision making systems, a method that will allow smaller companies to use LCA, and interoperable information models and standards to support a complete system. As detailed in the workshop, the critical challenges to developing and implementing a comprehensive methodology for sustainable product design include a structured design decision approach to simultaneously examine the economic, environmental, ethical and social issues associated with the lifecycle product design process, as well as a formal knowledge

representation framework to seamlessly capture and propagate information throughout the design process. Along these lines, NIST offers the most comprehensive approach by emphasizing the need for a Triple Bottom Line (TBL) assessment method of significant impacts [4]. This means that impacts on people, the planet, or profit should be considered. In doing so, the environment, the economy, and social welfare considerations that effect the population can not only be preserved over a long period of time, but it will also lead to a new paradigm for competitive product design. From the industry side, there is also a growing recognition that the minimization of the environmental impacts typically involves Life Cycle Impact Assessment (LCIA) methods to determine the specific inputs and outputs of environmental impact components. Ecoinvent, the world's leading supplier of consistent and transparent lifecycle inventory (LCI) data of known quality provides data implemented within sixteen different established methods [5]. Accordingly, software tools have been developed to automate the lifecycle assessment (LCA) process. For example, the software provided by Gabi and SimaPro [6] determine the environmental impacts of a specific product design. However, these software solutions lack consideration of the economic and society related objectives. More importantly, no such software solutions exist to enable sustainable product design, which requires a methodical multicriteria decision making methodology and a framework for its implementation with systematic knowledge representation.

It is then apparent that such a development will require fundamental research in two key areas: 1) A rational multicriteria decision making method for sustainable design to account for the different social, economic, and environmental considerations, and the developed method should be able to account for the uncertainties in the available data and the related assumptions. 2) The design information and knowledge necessary for design may come from across multiple organizations, companies, and countries. The study of engineering design as an iterative decision-making procedure in recent years has led to utilization of the concepts from decision analysis to solve engineering design problems [7]. Normative decision analysis principles provide valuable insights in advancing the state of knowledge on rational design decisions and enable a better

understanding of their consequences from an overall design perspective. From a practical point of view, decision-based design offers a formal strategy to reduce the multiple attributes in an engineering design problem to a single overall utility function in a probabilistic sense, which reflects the designer's intent and preferences under conditions of uncertainty [8]. Thurston and her associates had postulated a multi-attribute decision model for sustainable design and proposed a methodology for preference aggregation [9,10]. However, in spite of its proven track-record in other domains, the use of normative Multiple-Criteria Decision Making (MCDM) methods has been limited in sustainability studies. Specifically, there has been no detailed study on the development of decision-based design techniques to enable preference modeling and decision making under uncertainty. Further, measuring and ensuring consistent preferences is a critical issue that has not received full theoretical treatment in the literature. If multiple decision makers are expressing their preferences, being able to aggregate these preferences using a sound and rational method is needed. The efforts to develop such methods in the area of decision making in sustainable design have been compounded by a lack of standards for handling material and energy data at different phases of the designed product's life cycle.

A review by Ramani et al. [11] reinforces this assertion as it applies to facilitating the early stages of sustainable product design, including the representation of the LCA measures and their uncertainties. In a subsequent work, Ramani and associates propose the use of an information gap method for estimating the effects of the LCA uncertainties during product redesign [12]. How environmental knowledge modeling can further enhance the capabilities of sustainable product design and manufacturing has been detailed in a recent NIST study [13]. Along these lines, Dr. Kim and his associates have articulated the need to develop a semantic information model for lifecycle product design [14]. These studies recognize that design information and knowledge necessary for decision-based design may come from across multiple organizations, companies, and countries. Integrating distributed engineering information that allows decision makers to easily access and understand it is essential for making well informed

decisions. Therefore, appropriate models and simulation tools are necessary to predict results and optimize decision making in sustainable product design. Semantic information models that accurately represent all sustainability factors across all of the life cycle stages are crucial to enable decision making throughout the lifecycle design process. Such a model represents the integration of all relevant factors across the life cycle stages, as well as design solutions found from integrated optimization. The resulting knowledge management approach can enable documenting and seamlessly integrating distributed design knowledge during the evaluation of design alternatives. Such an approach should take advantage of emerging Semantic Web technologies to improve collaboration through increased understanding of content and representation of sustainability-related knowledge in a manner that is easily shareable and distributable.

CHAPTER 2

SUSTAINABILITY-BASED PRODUCT DESIGN

Addressing the above challenges, this research focuses on the identification and development of a decision support system for sustainable product design to reduce the multiple attributes to a single overall utility function in a probabilistic sense, which reflects the designer's intent and preferences under conditions of uncertainty. To facilitate consistency of design information at all stages of the product's life cycle analysis and to enable methodical comparison of the design alternatives, this work also develops a semantic web-based, collaborative approach for our decision-based design strategy. Here, this work extends the e-Design framework at UMass-Amherst [15-25] by integrating sustainable product design information within the semantic web to support knowledge management and information sharing throughout the entire design process. Here, the mathematical representation of the product design for sustainability can be framed as a multi-attribute optimization problem using Hypothetical Equivalents and Inequivalents Method (HEIM), which is a normative decision-based design method. The following sections highlight the main components of sustainable product design, and detail the key elements of this research. Most of the following six subsections appear in the published work¹ by Eddy et al. [46].

2.1. Life Cycle Assessment: Accounting for Life Cycle Inventory (LCI)

In a sustainable design process, the associated quantities of each environmental emission are obtained from established LCI data for each life cycle stage of each product component. The product lifecycle is normally comprised of five separate stages. All of

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the raw materials are first extracted and formed into the usable stock configuration. Next, the parts are manufactured and assembled as specified. Each of the parts and their materials emit their own set of environmental parameters, such as the grams of carbon dioxide, methane, or other substances emitted, during these first two stages. The finished product is transported to its point of use destination. The product is utilized in the intended fashion by the end user over the course of its lifetime. When the product is no longer usable or needed by the customer, it is either disposed of or recycled for future use. The end of life stage could lead to any of a number of scenarios depending upon what the product and its components are. Some products are disposed of in a landfill. Some products are designed for reuse in the next product generation by disassembly or modification in a modular fashion. In some cases, the parts of certain material types could be incinerated to form a recycled raw material for future manufacturing of other products.

The knowledge base of LCI data for each life cycle stage has been expanding over the recent years for greater transparency and accuracy as more information about environmental emissions becomes available for various materials, manufacturing processes, etc. The data and the means of applying it to determine environmental impacts have evolved from that originally prescribed by Wenzel et al. [26] in their book, which formally introduced the EDIP (Environmental Design of Industrial Products) program. More recently, the U.S. EPA developed TRACI (The Tool for the Reduction and Assessment of Chemical and other environmental Impacts) to implement a framework for decision making by characterizing the impacts determined from LCI data [27]. Our method uses the available current guidelines derived from TRACI and EDIP to express

the environmental parameters of chemicals emitted or resources depleted by a process in terms of the resulting specific environmental impacts.

2.2. Life Cycle Assessment (LCA) Strategies

The LCA process converts the environmental emissions determined from LCI data at all the lifecycle stages into environmental impacts over the complete product lifecycle. Environmental impact categories usually include: global warming, acidification, eutrophication, photochemical smog, ozone depletion, toxicity, and resource depletion. ISO 14040 calls for the LCIA (Life Cycle Impact Assessment) step to follow the inventory analysis step in an LCA process [28]. LCIA methods determine the specific inputs and outputs of environmental impact components.

After identifying the impact categories, ISO 14042 mandates that an LCIA process involves classification followed by characterization [29]. Classification establishes which emission quantities from LCI contribute to each impact category. Each emission parameter can contribute to more than one impact and each impact is often comprised of more than one parameter. Thus, characterization determines the relative impact of each parameter within each impact category. The inventory data is multiplied by the characterization factor to find each impact indicator. Each specific impact is the sum of all the indicators in that impact category. Tools with access to the ecoinvent database usually have both LCI data and the resulting characterization factors for application of the LCIA methods [5]. Tools such as the SimaPro software access the ecoinvent database [30].

Uncertainty in the LCI data warrants consideration. The ecoinvent database introduction document [31] provides simplified estimates of the geometric standard

deviation of the various environmental parameters. The uncertainty combined with the number of impact categories to compare pose significant challenges to finding the optimal alternative. A procedure was developed to simplify the comparison of the various environmental impacts [26,29]. This procedure employs the steps of normalizing, grouping, and weighting the impacts. All impacts are normalized to have the same units. Next, impacts are grouped into categories which allow direct comparisons of the contained impacts to each other. Finally, weights are applied to each impact based on the level of importance relative to each other. This helps to simplify the MCDM process. It should be noted that the data for our NASDOP methodology can thus directly be estimated from established databases.

2.3. Inclusion of the Cost Attribute

The triple bottom line objective mentioned earlier requires us to include more than just the environmental impacts in our MCDM optimization method. EIO – LCA (Economic Input-Output Life Cycle Assessment), developed at Carnegie Mellon, uses economic data on the aggregate level of the different sectors to estimate the dominant LCA impacts [32]. Here, correlations between economic and environmental data can overcome LCI data acquisition difficulties when a less accurate result may still be useful. Upon examination of the inclusion of LCC (Life Cycle Costing) with an LCA analysis, Schmidt [33] warns that uncertainties are higher in LCC than in LCA due to the effect of future costs and discounting rates over a product lifecycle, especially for end of life considerations. SimaPro documentation [30] identifies several challenges that have prevented the inclusion of cost information with LCA evaluations done by software. Such challenges include: the accuracy of discount rate determination, the accuracy of including

allocated overhead costs, and the accuracy requirements are more critical to an enterprise for cost, revenue, and profit. Alternatively, the software estimates liability costs due to noncompliance or a resulting loss of goodwill. The method presented in Chapter 5 addresses these challenges while including LCC and LCA attributes together in the same MCDM model to optimize toward the triple bottom line objective for sustainability.

2.4. Conceptual Design Strategies

The process to formulate the appropriate MCDM model for optimization during the conceptual design stage involves another key challenge. Formulation of this model needs to facilitate the identification of representative potential design alternatives. One approach to provide such guidance during conceptual design is the function impact matrix method, proposed by Devanathan et al. [34]. This method examines each category of a new product design to relate the functions to corresponding environmental impacts. Zhao et al. [35] address the marketing aspects of sustainable product design in terms of the need to align functionality with the voice of the customer as an important part of conceptual design beyond simply informing the design decision methodology. An extension of the traditional design process for DfE (Design for Environment) was proposed by Nielson and Wenzel [36]. Here, the LCA process is applied to a baseline design to find the most significant environmental impacts. Potential alternatives to the baseline design are identified and compared. The optimal among the design alternatives is selected to which the design details are developed. Since the alternatives are conceived of during conceptual design, the need to perform subsequent iterations of the design process may be revealed as the design details are developed. The review by Ramani et al. [11] asserted that few quantitative tools exist to use for DfE during conceptual design.

The main problems were identified as the cost of LCA and the lack of LCI data for new designs. The early design stages offer the greatest flexibility to make design improvements. Reap et al. [37,38] further expand upon a number of issues that can limit the practical use of both LCI data and LCA methods. Such issues include the accurate representation of uncertainty, the inclusion of LCC and social impacts for sustainable decision making, and the allocation of environmental flows to the appropriate process. The goal of this work is to address many of these challenging areas comprehensively through the development of needed methodologies. To this end, several pertinent research questions are formulated from the current challenges. First, how can sustainability objectives be considered efficiently at the conceptual early design stages without significant loss of either credible modeling of the physical reality or consideration of an entire design space? Furthermore, what method based on reasonable assumptions can be derived to simplify the high fidelity modeling of LCA for early design efficiency? Next, when and how can standards, or regulations, be modeled as constraints in a constrained optimization model without sacrificing the mathematical rigor of the normative construction of a multi-criteria decision making problem? Finally, when can modeling of an entire design space reveal more optimal solutions that do not currently exist, such as the requirements for a new material that does not exist yet?

To address these important research questions, the relevant work is presented in Chapters 5 through 7. The following two chapters identify the bases on which these works were developed.

CHAPTER 3

NORMATIVE DECISION ANALYSIS

3.1. Problem Formulation

Our method is based on the fundamentals of normative decision analysis [7]. Dr. Howard's work [39-41] formed the fundamental basis of its use for systems engineering. These normative techniques use expected utility theory, which consists of the three main components of options, expectations and value. Here, the decision rule requires the preferred option be that with the expectation of the highest value, or utility. The premise is that real-valued functions can represent the preference structure, which can determine the maximum, or most desirable, utility value of a design by using a normative analytical method [42]. The technique has the five major steps [42] of: (1) identification of the significant design attributes and generation of the design alternatives (2) verification of relevant attribute independence conditions (3) evaluation of the single-attribute utility (SAU) functions and the preferences of each relative to each other (4) aggregation of the SAU function into a single multi-attribute utility (MAU) function, which represents the complete system (5) selection of the alternative with the highest MAU value by rank ordering the alternatives.

In other words, each attribute or objective has a normalized utility value ranging from 0 to 1 corresponding to the worst possible attribute value and the best possible value, respectively. The preference structure of each monotonic SAU function can be established by articulation of the certainty equivalent, at which value a decision maker is indifferent to a lottery between the best and worst possible values [7]. The MAU function for each alternative consists of a linear function with a computed value equal to the sum of the products of every attribute's utility value and the attribute's preference weight value. The sum of all attribute weight values is equal to 1. The method by which each attribute's weight is determined to accurately model the preference of a decision maker is summarized in the following section.

3.2. HEIM - Hypothetical Equivalents and Inequivalents Method:

Execution of this solution is best accomplished by an accurate and computationally efficient decision model. HEIM (Hypothetical Equivalents and Inequivalents Method) was developed for such cases that involve selection from among multiple attributes having various advantages and disadvantages. The advantages of HEIM were demonstrated in the selection of the optimal aircraft for an entire airline fleet given the tradeoffs of the maximum speed, the maximum nonstop cruise range, and the number of passengers that may be seated [43,44]. This method has the capability of consistently modeling the preferences expressed to detect any rank reversal issues. Here, hypothetical alternatives are assigned standardized and normalized utility values for each attribute. This way, the complete design space is represented by an experimental design to minimize computation.

A prior study [45] deployed a three level L_9 orthogonal array to solve a design problem with three attributes. The standard utility values in each cell correspond to the normalized most desirable, least desirable, and mid-level of desirability for each single attribute. Thus, the attribute values at each standard level correspond to single attribute utility values of 1 (most desirable outcome), 0 (least desirable outcome), and 0.5. The 0.5 utility values correspond to the risk preferences expressed by the decision maker for each individual attribute. In this case, ranking of the nine hypothetical alternatives by a decision maker could establish the decision maker's preferences for the formulation of the MAU function. Table 1 shows the construction of the three level L_9 orthogonal array that is used to solve for the three weights of a three attribute design selection problem. The three level L_9 orthogonal array, with nine hypothetical alternatives, was selected for a three-attribute problem to completely define the attribute space with order and balance [45] while also minimizing the number of hypothetical alternatives needed. Here, we see that each hypothetical alternative has a MAU value that is a function of the three weights. When a decision maker ranks these nine hypothetical alternatives, inequality constraint equations are established for each comparison. For example, if hypothetical alternative C were preferred to

hypothetical alternative B, then it must also be true that $w_1 + w_2 + 0.5w_3 > 0.5w_1 + 0.5w_2 + w_3$.

Since the sum of the weights must equal 1, HEIM determines the weights by solving the optimization problem of:

$$\text{Minimize } f(x) = \left(1 - \sum_{i=1}^n w_i\right)^2 \quad (1)$$

$$\text{Subject to the constraints of: } g(x) \leq 0, \quad (2)$$

where x is the vector of attribute weights, n is the number of attributes, and w_i is the weight of attribute i [45]. It should be noted that HEIM procedure also enables a consistency check of the designer's stated preferences for the avoidance of rank reversal issues. The effectiveness of HEIM to optimize traditional engineering design solutions was demonstrated in prior research [45]. Thus, our new method needs to effectively simplify a sustainable design formulation into a form to which HEIM or other normative methods may be applied effectively and efficiently.

Table 1: Hypothetical alternatives using an L_9 orthogonal array [45]

Hypothetical alternative	Attribute 1	Attribute 2	Attribute 3	Value of alternative
A	0	0	0	0
B	0.5	0.5	1	$0.5w_1 + 0.5w_2 + w_3$
C	1	1	0.5	$w_1 + w_2 + 0.5w_3$
D	0	0.5	0.5	$0.5w_2 + 0.5w_3$
E	0.5	1	0	$0.5w_1 + w_2$
F	1	0	1	$w_1 + w_3$
G	0	1	1	$w_2 + w_3$
H	0.5	0	0.5	$0.5w_1 + 0.5w_3$
I	1	0.5	0	$w_1 + 0.5w_2$

CHAPTER 4

A SEMANTIC FRAMEWORK FOR SUSTAINABLE PRODUCT DESIGN

Representation of such a method is best accomplished with a collaborative Web-based environment for improving communication by formally defining a platform for documentation and sharing of engineering design knowledge throughout the entire design process [15-25]. The research group at UMass –Amherst’s Center for e-Design established an e-Design framework through an ontological structure to concisely define a set of individual engineering concepts. A library of modular ontologies for engineering design has been developed and a customized ontological knowledge-base has been established to enable linking of the modular ontologies together in a semantic web environment. The set of modular ontologies linked together create a flexible, yet consistent, product development knowledge-base.

The resulting e-Design infrastructure uniquely enables the information stored within the knowledge-base to be readily inspectable and computable, thus allowing for design tools that reason on the information to assist designers and automate design processes. This ontological

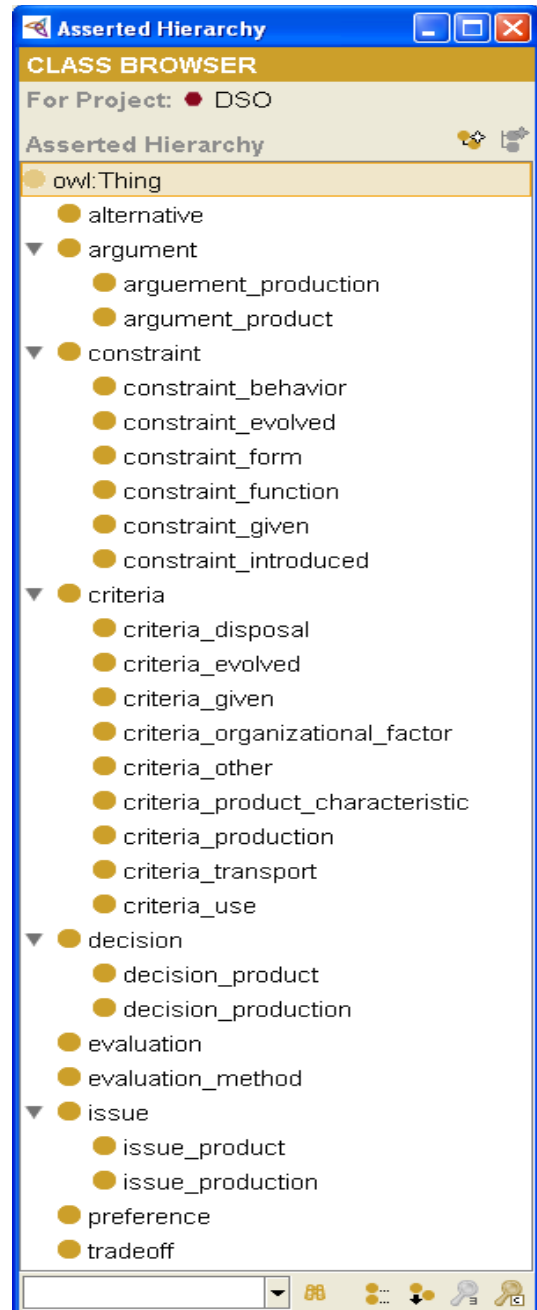


Figure 1: Decision Support Class Hierarchy

knowledge-base can be used to prompt engineers to document important product development information, increase understanding of the design process, provide a means to intuitively retrieve information, and seamlessly access distributed information. The ontologies were developed in OWL format and created with appropriate class structures with relevant properties to build upon for a range of concepts in sustainable product design. Key concepts in the decision support system for the sustainable product design ontology include semantic information from design alternatives to decisions to methods used to LCA features etc. For example, Figure 1 shows the resulting class hierarchy in the ontological decision support system and Table 2 shows the generic information that can be captured for the decision class.

Table 2: Semantic information for the decision class

<i>Property</i>	Type	Description
has evaluation method	Object	Specifies the decision method used to make the decision
for issue	Object	Specifies the issue being addressed
has evaluation	Object	Specifies the evaluation information used in this decision
selected alternative	Object	Specifies the alternative chosen to resolve the issue
decision summary	Data	Text that provides a brief summary of the decision made
tradeoff considered	Object	Specifies a tradeoff that was involved in this decision. The tradeoff must occur between objective parameters identified in the preference model
has evaluation method	Object	Specifies the specific evaluation method used
decision outcome	Data	Qualitative evaluation of how well the selected alternative addressed the issue
comment	Data	States any additional thoughts that the decision maker considers relevant and important

CHAPTER 5

NASDOP: NORMATIVE DECISION ANALYSIS METHOD FOR THE SUSTAINABILITY-BASED DESIGN OF PRODUCTS

This chapter presents the published work² by Eddy et al. [46]. The work introduces a novel fundamental methodology to consider quantified utility maximization of environmental and economic attributes based on the stated preferences of a designer over a complete product life cycle. In this approach, actual measurable flows of the environmental and economic factors are determined, along with their uncertainties. The architecture of this NASDOP method is constructed within a normative decision-based framework to enable consistent modeling of the mean expected and worst case resulting attribute values and their corresponding single-attribute utility (SAU) functions and composite multi-attribute utility (MAU) functions of discrete alternative design instances. The following sections describe the components of this architecture, which is illustrated in the final sections of this chapter by the results of an actual case study.

5.1. NASDOP Architecture

Figure 2 below outlines the NASDOP (Normative decision Analysis method for the Sustainability-based Design of Products) design process including life cycle assessment and the associated costs. First, we illustrate the use of NASDOP during the early stages of conceptual design. Here, various potential design goals and alternatives are established for comparison. For each design alternative, including a baseline design, LCA and LCC are used to account for all environmental and cost flows to determine the resulting environmental and cost attributes. Since the uncertainty in environmental and cost data is significant, it is important to also account for the uncertainties and represent the variability in the analysis. Then, HEIM is executed to find the weights of the attributes based on the stated preferences of the decision maker. Next, the MAU values are computed for each design alternative and the alternative with the greatest MAU value

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is chosen. The following sections detail the various steps and highlight the unique aspects of NASDOP.

5.1.1. Identify Design Alternatives and State Assumptions

The alternatives, at the initial three stages shown in Figure 2, would be based on assumptions regarding the results. Here, for illustrative purposes, design alternatives are identified for comparison to each other to show how the methodology evaluates different designs quantitatively. This method is further developed as described in Chapter 7 to determine optimal solutions using surrogate modeling that can search the entire design space for a global optimal point in the feasible region given the weights determined by HEIM to find that single optimal point on the Pareto optimal solution set.



Figure 2: Design process for sustainability using NASDOP

Feasibility constraints may depend upon other design goals. For example, a design would need to satisfy certain functional and reliability requirements in addition to the optimization of the sustainability objectives. The best of these alternatives in this illustration is selected during the MCDM analysis. As the design process progresses, the selected alternative is developed by more detailed engineering analysis. The increased knowledge about the solution may validate all of the original assumptions made during the conceptual design, but it could also reveal that one or more of the original requirements cannot be met. If an assumption is not met, the design process requires an additional iteration. Table 3 illustrates an example of assumptions that may be made about alternatives to compare during conceptual design for the sustainable design of some

product. Of course, the assumptions and goals or any feasibility constraints will vary depending upon what product is being designed. This method could be equally applicable to a different set of constraints for different products and different specifications.

Table 3: Possible assumptions for alternatives

Alternative #	Description of Strategy	Specific Design Goal
X1	Weight reduction [47,48]	15 % reduction of all component weights
X2	Use recycled material [47,48]	100 % recycling at the fifth lifecycle stage
X3	Reduce the energy content [47,48]	18 % reduction in manufacturing impacts and 12 % reduction in raw materials' impact
X4	Low toxicity	35 % reduction of all impacts except for resources depletion and cost
X5	Less nonrenewable resources	50 % more recycling at the fifth stage; natural gas effects on the greenhouse gas impact and all of the impacts due to resources consumed are both cut in half
X6	Modify for more energy efficient use [47,48]	1/3 less energy during the product use stage but adds 2 % to all material and manufacturing impacts due to additional components
X7	Manufacturing impact reduction	25 % reduction in manufacturing stage impacts

Representation of the goals in the third column of Table 3 requires modification to the baseline calculations for each alternative of the various objective attributes. One such attribute is the cost. The NASDOP enables systematic accounting for the economic impacts as well as the environmental impacts of any product design.

5.1.2. Account for Flows

Flows to be considered for environmental considerations consist of material emissions as well as energy and resource consumption. The flows for economic considerations pertain to

monetary costs throughout the lifecycle of the product. Although the data source and type is very different for LCI and LCC, we can show that the formulations used to compute the LCC impact at each stage are very similar to that used during the LCA process to find the environmental impacts. Furthermore, the LCC function conveniently depends upon the same independent variables as do the LCA impact functions, aside from the different data source. LCC is actually simpler and requires less computation than LCA in that it depends upon only a single monetary parameter instead of nearly a dozen (or more for some products) LCI parameters that describe multiple sources of emissions. Thus, classification, grouping, and characterization are not necessary to compute LCC impacts whereas LCA impact computations require all of these additional steps. Furthermore, the derived expressions to calculate the lifecycle cost are directly compatible with the formulas previously deduced to calculate the LCA impacts [48]. The expressions that we derived to calculate the lifecycle costs at each of the five product lifecycle stages are shown in the following equations. The proposed method would be equally applicable if additional factors were included such as different percentages for end of life dispositions or greater detail from the sources of cost allocations.

Equation (3) formulates the life cycle costs for the first stage of raw material extraction.

The cost per unit is given by

$$\phi_1 = \sum_{i=1}^{n-parts} \frac{(\alpha_{i1} \Lambda_i)}{\gamma} \quad (3)$$

where α_{i1} is material cost per gram of part i, Λ_i is weight in grams of part i, and γ is the mass inclusion factor of parts considered. This is the weight percentage of the total weight represented by those parts included in the computations. Equation (4) formulates the life cycle costs for the second stage of manufacturing. The cost per unit for that stage is given by

$$\varphi_2 = \left(\sum_{i=1}^{n-parts} \frac{(\alpha_{i2} \Omega_i)}{\gamma kW_i} \right)_{parts} + \left(\frac{\alpha_2 \Omega}{kW} \right)_{Assembly} \quad (4)$$

where α_{i2} is the cost per hour to manufacture part i, α_2 is the cost per hour to assemble all manufactured parts together, Ω_i is the kilowatt-hours consumed to manufacture part i, γ is the mass inclusion factor of the parts considered, and kW_i is the kilowatt demand of the manufacturing process. Equation (5) formulates the costs for the third stage of distribution. The cost per unit due to distribution is given by

$$\varphi_3 = \alpha_3 \Delta \theta \quad (5)$$

where α_3 is the cost per ton of product weight per km traveled, Δ is the km travelled, and θ is the product weight in tons. Equation (6) formulates the costs for the fourth stage of product use for a case where energy consumption is the main cost incurred. The costs per unit during such a product use scenario is given by

$$\varphi_4 = (\alpha_4 \Phi + \beta_4) N \quad (6)$$

where α_4 is the cost per kilowatt-hour, Φ is the kilowatt-hour per use, N is the number of uses per product lifetime, and β_4 is any additional cost per use, which is product dependent. Equation (7) formulates the costs for the final life cycle stage of end of life disposition. The costs per unit due to end of life processes is given by

$$\varphi_5 = \sum_{i=1}^{n-parts} \left(\sum_{k=1}^3 \Pi_{ik} \alpha_{ik5} \right) \Lambda_i \quad (7)$$

where α_{ik5} is the net cost of disposal or reuse per kg of weight of part i with kth end of life option, which can be negative for a net positive reuse cost avoidance, Λ_i is the weight of part i in kilograms, Π_{ik} is the per cent rate of ith part with kth end of life option. For the landfill part end of life scenario, k is equal to one. For incineration part end of life scenario, k is equal to two. For

recycling part end of life scenario, k is equal to three. Here, the following scenarios are assumed: Metals are 60% recycled and 40% incinerated. Cardboard packaging is 50% recycled and 50% landfill. Plastic is 70% landfill and 30% incinerated [48]. Equation (8) shows the Life Cycle Cost (LCC) objective function to minimize and is given by

$$f_{\text{cost}} = \sum_{i=1}^5 \Phi_i \quad (8)$$

5.1.3. Account for Uncertainties

Having computed the mean values of the environmental and cost impacts, it is equally important to account for any significant variability in the values. As mentioned previously, levels of uncertainty are significant in both environmental and economic lifecycle computations. In order to accurately compare the various design alternatives, we ought to account for any significant sources of uncertainty. The existence of uncertainty means that actual values range probabilistically between minimum and maximum values. The data input to calculations is a significant source of uncertainty for both environmental impacts [31] and also for economic impact due to price volatility [49]. Some additional uncertainty may also result from the accuracy of characterization, normalization, and weighting factors under various situations. A prior study shows that LCI data is the most significant source of the uncertainty and newer LCIA methods of applying the weighting factors, such as Eco-indicator 99, have less uncertainty than does the earlier adopted EDIP method [50]. Additional sources of uncertainty could also affect the lifecycle cost as described previously. Here, we assume that the data sources account for the most significant amount of uncertainty. The ecoinvent database introduction document [31] provides a simplified source of information to account for the most significant source of uncertainty. Here, other data quality issues such as reliability, completeness, and temporal and geographic variability are accounted for by a discrete range of additional uncertainty factors, which may also contribute to account for any of the other uncertainty sources. This way, a composite geometric

standard deviation is determined to account for the multiple uncertainty sources. This also has relevance to cost uncertainty. However, note that the data quality uncertainty of cost is more dependent upon the maturity of the cost information within an enterprise, whereas data quality uncertainty of environmental parameters depends more so upon the development of the applicable LCI data and LCA factors according to the ISO 14042 guidelines, which is often provided by a

Table 4: Geometric standard deviations of data uncertainty

Environmental Parameter (or cost)	Basic Uncertainty Factor [31]	GSD (Geometric Standard Deviation) (d) [31]
CO2	1.05	1.13 (b)
NO x	1.5	1.26 (b)
Methane	1.5	1.26 (b)
CO	5.0	2.26 (b)
SO2	1.05	1.13 (b)
VOC	1.5	1.26 (b)
Resource depletion	1.75 est.	1.35 est. (b)
Monetary Cost	1.15 (a)	1.68 (c)

a – This is calculated from the example of the price uncertainty of an annual fuel price standard deviation of +/-7.75% and assuming a 4 year average product lifetime and normally distributed geometric Brownian Motion [49]. This number changes from 1.15 to 1.30 if the product lifespan is 15 years.

b – This assumes middle data quality level for LCA.

c - This assumes below mid-level data quality for cost until a verified data source is found or established over time.

d – The formula for Geometric Standard Deviation (GSD) is given by

$$GSD = \sqrt{\exp\left(\ln(U_1)^2 + \ln(U_2)^2 + \ln(U_3)^2 + \ln(U_4)^2 + \ln(U_5)^2 + \ln(U_6)^2 + \ln(U_b)^2\right)} \quad (9)$$

where U_1 is the uncertainty factor of reliability, U_2 is the uncertainty factor of completeness, U_3 is the uncertainty factor of temporal correlation, U_4 is the uncertainty factor of geographic correlation, U_5 is the uncertainty factor of other technological correlation, U_6 is the uncertainty factor of sample size, and U_b is the basic uncertainty factor. [31]

third party source. Environmental data has been found to be log-normally distributed [31]. Table 4 shows a summary of the resulting quantitative measures that allow us to represent all relevant uncertainties as given by log-normally distributed data [31]. Here, we assume that data has an average or middle level of environmental data quality. Each mean expected value given by LCI

data combined with the calculated geometric standard deviation given in Table 4 provides enough information to calculate the standard deviation and the resulting 95% confidence interval upper and lower limits of each environmental parameter. Thus, the upper and lower limits of the 95% confidence interval can be calculated for each environmental impact as well as for the lifecycle cost. This information is needed to determine the highest and lowest possible outcomes for each attribute value in the MCDM model. Now that each attribute value for each alternative is calculated, both in terms of its expected values and probabilistic distributions, this information can be deployed within a decision model to identify the best of the alternatives.

5.1.4. Execute HEIM and Select the Best Alternative

Table 5 shows the sustainable product design optimization problem expressed in a structure consistent with the principles of normative decision analysis. Here, multiple attributes are listed that include the main environmental impacts and lifecycle cost. This allows comparison of a number of possible design alternatives to find the best of the identified alternative choices with the maximum MAU value. Thus, the solution of the multi-attribute problem involves the optimization of the composite function of all attributes subject to the compliance constraints. Each attribute value for each design alternative, X_j , depends upon the data values associated with the set of independent design variables, x_i , that comprise a given alternative. The objective functions $f_1(x)$ to $f_6(x)$ are equivalent to the environmental impacts, which are solved by applying the LCA process over all of the five life cycle stages. Each environmental impact is the linear sum of the products of each for related emission load and its characterization factor for that impact. Emission loads are calculated from LCI data corresponding to the design variables using the pertinent formula at each life cycle stage.

Having calculated all of the high, low, and mean values of the 95% confidence interval for each objective function, the formulation may be simplified by the way of minimizing the number of objective functions that need to be included in our MCDM model. To this end, we use the

LCA steps of normalizing, grouping, and weighting described previously [26,29] to directly compare the attributes of environmental impacts to each other. Initially, each impact is expressed in units of a kilogram equivalent quantity of a certain chemical compound. Since each impact is measured by a different chemical equivalent, normalization converts all impacts into the same units. The normalized unit of milli-person-equivalent (mPE) is obtained for each impact by multiplying the kilogram equivalent value by the appropriate scaling constant used in prior case study examples [26]. Both environmental impacts and kilogram equivalent values of nonrenewable resources consumed may be expressed in mPE units. However, environmental impacts and resources depleted cannot be compared directly at the weighting step of LCA and must be grouped separately. Once they are grouped separately, the groups themselves can then be subsequently studied and evaluated as a MCDM process using HEIM. As mentioned previously, each impact must be weighted based on its relative importance to allow direct comparison to the other impacts. The scaling constants to convert to weighted units of milli-people equivalents targeted (mPET) for environmental impacts and milli-person-reserves (mPR) for resource consumption are taken from those used in prior case study examples [26]. From the sustainability perspective, an attribute with a significantly higher mPET or mPR value for any other attribute under consideration in the group will present the greatest priority for minimization among all attributes in its group. From the discussion, it can be concluded that a typical design for sustainability problem will have three major attributes, namely, the cost, environmental impact, and nonrenewable resource consumption. However, there can be several sub-attributes within the environmental impact and resource consumption attribute groups as well. The preference among the three major attributes is modeled using HEIM as shown in Section 3.2. The development of the decision model and the considerations for inclusion of attributes are illustrated with the aid of an actual case study to which the NASDOP is applied.

Table 5. Mathematical model for sustainable product design

<p>Maximize: $\Omega = \{f_1(\bar{x}), \dots, f_p(\bar{x})\}$, where $\bar{x} = (x_1, \dots, x_n)$</p> <p>Representative independent design variables: $x_1 \dots$ = Material types; $x_2 \dots$ = Manufacturing processes employed x_3 = Mode of Distribution employed; x_4 = Functional Priority x_5 = End of Life (EOL) Disposition; $x_6 \dots$ = Part Volume (due to the geometry of the part)</p> <p>Subject to: $g_k(\bar{x}) \leq 0 \quad \forall k$ Compliance constraints</p> <p>Select outcome from alternative set: $X = \{X_1, X_2, X_3, \dots, X_m\}$</p> <p>Representative attributes to minimize: $f_1(\bar{x})$ = Global Warming Potential (GWP) = kg CO_2 eq $f_2(\bar{x})$ = Acidification = kg SO_2 eq $f_3(\bar{x})$ = Eutrophication = kg NO_2 eq $f_4(\bar{x})$ = Photochemical Smog (ozone formation) = kg C_2H_4 eq $f_5(\bar{x})$ = Stratospheric Ozone Depletion = kg $CFC - 11$ eq $f_6(\bar{x})$ = Terrestrial Toxicity = LC_{50} eq [29] $f_7(\bar{x})$ = Aquatic Toxicity = LC_{50} eq [29] $f_8(\bar{x})$ = Human Health = LC_{50} eq [29] $f_9(\bar{x}) \dots$ = Resource Depletion = kg natural resources consumed eq $f_{10}(\bar{x})$ = Cost = USD</p>
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5.2. Case Study: Charcoal Grill

For illustrative purposes, the NASDOP approach is applied to the charcoal grill study used by Choi et al. [47,48]. Since Choi et al. [47,48] employed a descriptive method using AHP (the analytic hierarchy process), it provides a baseline case study to test our methodology. For this problem, the mean values are generated using the LCA methods described previously. Here, environmental loads for each of the six most significant parts in the charcoal grill are determined during the raw material extraction, manufacturing, and end of life stages of the product lifecycle. In addition, environmental loads are determined for the assembly of the complete product, for its distribution assumed average distance to a point of use, and for all uses of burning the charcoal briquettes over the course of the product's lifetime. Each environmental load is composed of all significant environmental emissions or non-renewable resources depleted during the operation.

Each environmental emissions load is calculated from the LCI data provided in the original study [47,48] with a mass inclusion factor to estimate the effect of all of the parts. The environmental impacts are next calculated as the linear sum of the products of each related emissions load and its characterization factor for that impact. The resulting mean values obtained for the eight significant environmental impacts agree closely with those published by Choi et al. [47,48]. From here, the NASDOP design approach is introduced to develop the decision model based on HEIM. The following sections detail the systematic development of rigorous mathematical models, as well as the methodical comparison of design alternatives to optimize for sustainability, while considering uncertainty in the economic and environmental data.

5.2.1. Potential Design Alternatives and Estimation of Flows and Uncertainties

Beyond the calculation of the baseline mean values, the NASDOP proceeds with the potential design alternatives and the calculation of flows and uncertainties for each design alternative goal. As stated in section 5.1.1, such alternatives can be identified according to the strategic goals specified back in Table 3. In this case, a decision matrix can be constructed with rows consisting of the complete alternative set and nine columns corresponding to the attributes under consideration. These nine attributes include one column for the cost, four sub-columns for the four different environmental impacts, and four sub-columns for the four different nonrenewable resources being consumed. Each of these columns has three sub-columns to also include the low and high values of each range covering the 95% confidence interval based on uncertainty. All resulting rows and columns with their calculated values in each cell are shown in Table A.1 of the Appendix. Once the calculations are completed to map design alternatives and design attributes, the attributes are normalized to have the same units with the exception of the cost attribute.

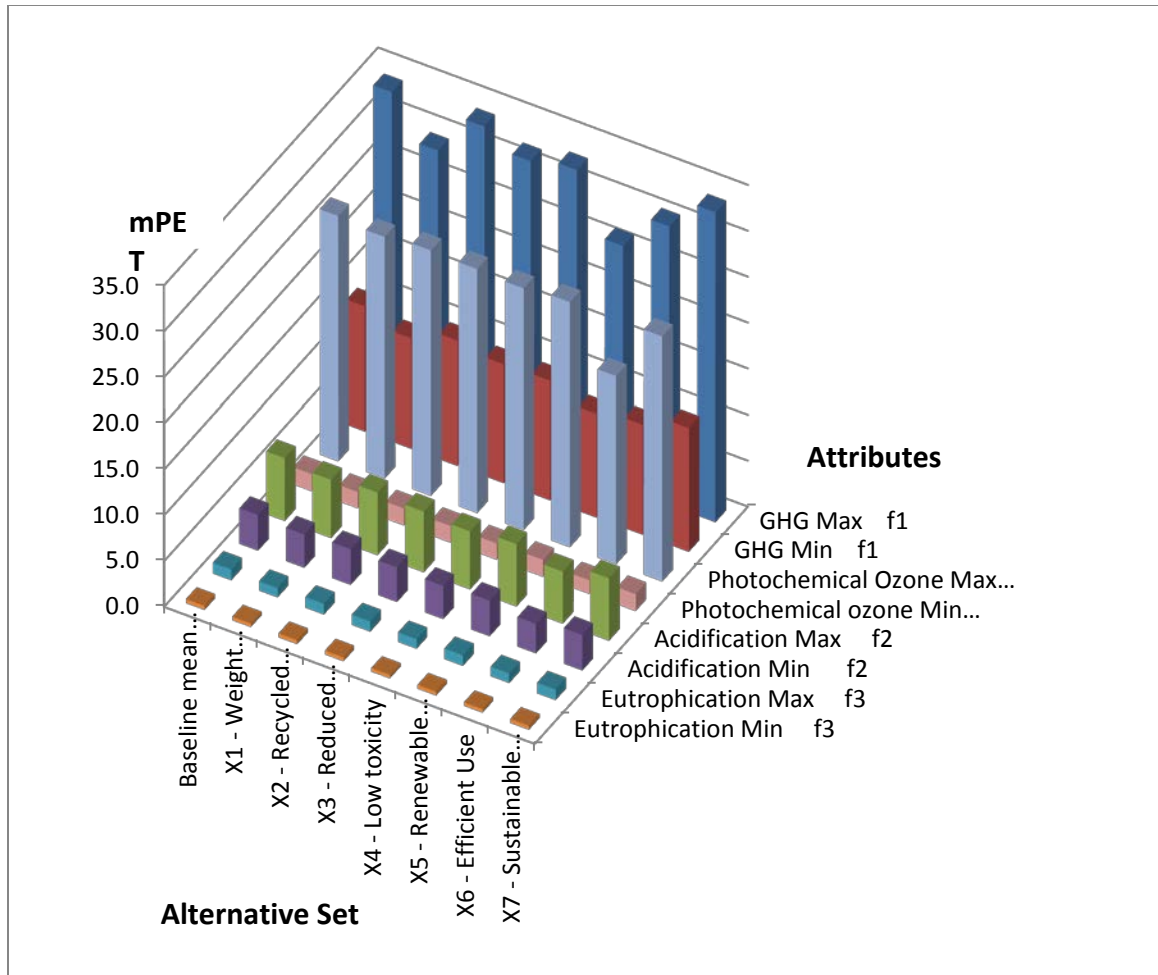


Figure 3: High and low values of environmental impacts weighted for direct comparisons

5.2.2. HEIM Results

The grouping and weighting procedures of LCA allow direct comparison of the four environmental impact sub-attributes to each other and a similar comparison of the four sub-attributes within the resource consumption grouping. Figure 3 shows the high and low weighted values of the four different environmental impacts. This illustration shows that some of these sub-attributes are more significant than others. The attributes have now been weighted using the LCA process based on their importance or severity relative to each other. These weights were determined by LCA development experts [26] based on the relative severity of each impact to the planet's sustainability. Recall that impacts are compared directly to each other based on the

measure of milli-people equivalents targeted (mPET). By the definition of sustainability, we will be most interested in reducing the impact that always has a higher value to a level that is closer to the value of the next most significant attribute. Figure 4 shows a similar weighted grouping for the depletion of nonrenewable resources.

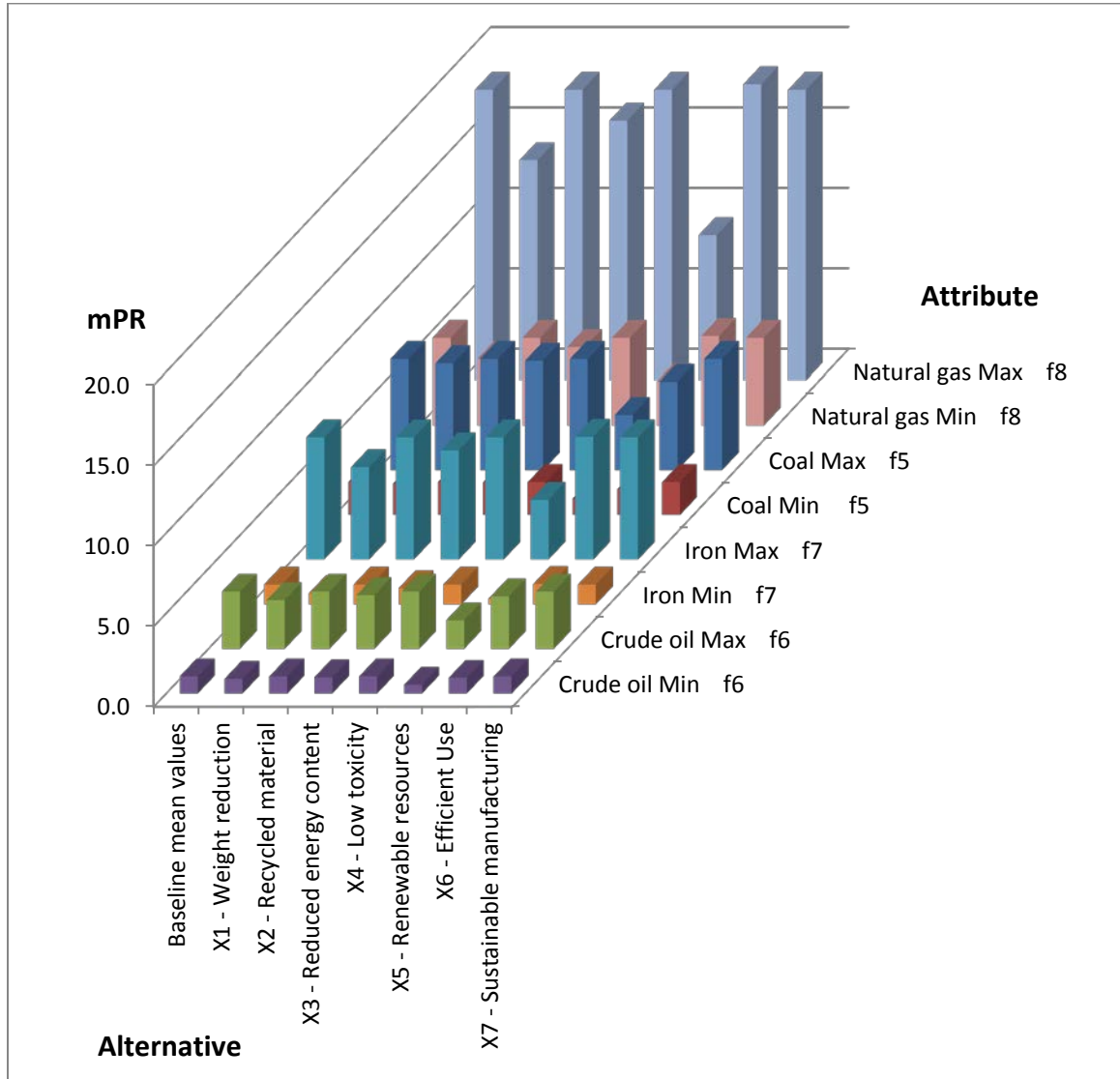


Figure 4: Nonrenewable resource consumption weighted for direct comparisons

The deployment of the weighting and grouping procedures from the LCA process generates the three-attribute model to execute within HEIM as described in Section 3.2. This construction is shown by the L_9 orthogonal array in Table 6. Here, we focus only on comparing the preferences among the three main groups by ranking the nine different hypothetical alternatives based on a decision maker's preference. A solution for such a three-attribute problem using HEIM was demonstrated in prior work [45]. The values shown in Table 6 correspond to the best (at $u=1$), worst (at $u=0$), and the certainty equivalent (at $u=0.5$) values. Here, the best and worst values represent the limits of the 95% confidence interval for the most critical attribute in the attribute group. Table 6 reveals that our first attempt to rank these hypothetical alternatives resulted in

Table 6: Hypothetical alternatives set up for the three-attribute case

Hypothetical Alternative	Critical Environmental Impact [mPET] f1	Critical Non-renewable Resource Depletion [mPR] f2	Monetary Life Cycle Cost [USD] f3	Possible Alternative Rank First Attempt	Corrected Alternative Rank
A	33.7	18.4	743	9	9
B	24.9	13.8	50	2	3
C	11.3	2.71	383	1	1
D	33.7	13.8	383	8	8
E	24.9	2.71	743	6	6
F	11.3	18.4	50	3	2
G	33.7	2.71	50	7	7
H	24.9	18.4	383	4	5
I	11.3	13.8	743	5	4

infeasible ranks of alternatives B and H. These rankings were not feasible, because the constraints imposed by such a ranking priority allow for no possible solution for the weights to use in a MAU function that will satisfy such a ranking of B and H. This was corrected by a ranking adjustment of these hypothetical alternatives as shown in the final column. The solution for the attributes'

weights given the preference defined by this ranking is {0.571, 0.143, 0.286}. Different decision makers may state different preferences during this process. This solution for the weights will be used to solve for the MAU values for each design alternative as described in the remainder of this section.

Since sub-attributes within the groups have already been weighted based on severity relative to each other, to optimize for sustainability, we may prioritize the reduction of the most significant impact value in each group. However, the uncertainty poses a challenging question to determine which impact has the highest value and whether we should compare the impacts based on their expected values or the values on the upper limit of their 95% confidence intervals. One approach could be to find the optimal alternative for both scenarios and see if the selected alternative is the same in both cases.

Tables 7 and 8 show the results of both approaches for this case. To obtain the utility values for each attribute in each alternative, we first had to establish the designer's preference for each attribute independently based on the risk preference for that single attribute. In this case, we assumed slightly risk prone decision making for monetary cost and risk aversion tendencies for decisions involving all of the environmental attributes. This can be seen in Table 6. The certainty equivalent (at $u=0.5$) values in all three attribute columns are not the average of the two extreme values. Each SAU function defined by the best, worst, and certainty equivalent values is used to find the utility value for each attribute value as shown in Tables 7 and 8. Note that the design process is equally valid and applicable for any and all preference sets as indicated by the designer. It is interesting that the two different approaches presented in Tables 7 and 8 resulted in the selection of two different design alternative goals. The approach shown in Table 7 does not consider the potential variations due to uncertainty and merely considers the expected values. When this approach of disregarding the uncertainty is used the design goal of choice with these stated preferences becomes the design of a product that consumes less energy during use. However, Table 8 shows that the design alternative of choice changes to the goal of designing a

Table 7: Design alternative selection based on the mean expected values

Design alternatives	Expected mean values					Expected mean utility values, u			Total utility value, U
	Environmental impacts [mPET] f1		Non-renewable resource depletion [mPR] f2		Monetary cost [USD] f3	Environmental impacts f1	Non-renewable resource depletion f2	Monetary cost f3	
	Value	Critical attribute	Value	Critical attribute					
Baseline mean values	21.3	GHG	10.35	Natural gas	246	0.661	0.735	0.701	0.683
X1 - Weight reduction	19.9	GHG	9.01	Natural gas	240	0.717	0.801	0.710	0.727
X2 - Recycled material	21.2	GHG	10.28	Natural gas	225	0.665	0.738	0.732	0.695
X3 - Reduced energy content	20.1	GHG	9.25	Natural gas	232	0.709	0.790	0.722	0.724
X4 - Low toxicity	20.6	GHG	10.35	Natural gas	246	0.689	0.735	0.701	0.699
X5 - Renewable resources	17.1	GHG	5.17	Natural gas	233	0.689	0.940	0.720	0.734
X6 - Efficient use	19.1	GHG	10.54	Natural gas	207	0.748	0.724	0.759	0.748
X7 - Sustainable manufacturing	21.3	GHG	10.35	Natural gas	234	0.661	0.735	0.719	0.688
Max U = 0.748									

Table 8: Design alternative selection based on the high limits of the confidence interval

Design alternatives	High limit values of 95% CI					High limit utility values, u, of 95% CI			Total utility value, U
	Environmental impacts [mPET] f1		Non-renewable resource depletion [mPR] f2		Monetary cost [USD] f3	Environmental impacts f1	Non-renewable resource depletion f2	Monetary cost f3	
	Value	Critical attribute	Value	Critical attribute					
Baseline mean values	33.7	GHG	18.03	Natural gas	743	0.000	0.049	0.000	0.007
X1 - Weight reduction	29.2	GHG	13.68	Natural gas	724	0.279	0.514	0.025	0.240
X2 - Recycled material	33.7	GHG	18.03	Natural gas	722	0.000	0.049	0.023	0.014
X3 - Reduced energy content	31.8	GHG	16.12	Natural gas	702	0.124	0.284	0.055	0.127
X4 - Low toxicity	32.7	GHG	18.03	Natural gas	743	0.066	0.049	0.000	0.045
X5 - Renewable resources	26.7	Photochemical ozone	9.01	Natural gas	730	0.414	0.801	0.017	0.356
X6 - Efficient use	30.3	GHG	18.38	Natural gas	632	0.215	0.000	0.150	0.166
X7 - Sustainable manufacturing	33.7	GHG	18.03	Natural gas	710	0.000	0.049	0.044	0.020
Max U = 0.356									

product that uses less non-renewable resources during its life cycle when the focus of concern shifts to mitigation of the worst case scenario possibility. Thus, the effects of uncertainty can directly influence the selected design alternative as can changes in the preferences stated by the decision maker.

5.3. NASDOP Discussion

The results show that NASDOP offers an effective and comprehensive methodology to design for sustainability in a manner consistent with the principles of the triple bottom line. To further examine its effectiveness, we considered quantifiable triple bottom line objectives and a mathematical model suitable for a normative solution. As detailed below, we were able to directly integrate the information from LCA as required by ISO 14042, account for all significant uncertainty, develop a mathematical preference-consistent decision support model from the entire design process perspective, including conceptual design.

The triple bottom line objectives include any and all impacts on the environment, economy, and society. Our method accounts for such effects on the environment and the economy. Future work can also examine societal considerations, which are not quantified as seamlessly. Chapter 7 provides an approach to express such metrics as they relate to performance objectives of importance to stakeholders and customers. The development of usable metrics to represent the most important societal considerations remains a topic of research. One such metric, which was represented quantitatively in the case studies by Wenzel et al. [26], accounts for the impacts of the probability of work place injuries during the processes involved in a product lifecycle. Ideally, the objectives should both accurately account for the metric and depend functionally upon the same independent variables as much as possible. The formulas that we deduced to compute the LCC impacts, which are presented in section 5.1.2 of this chapter, meet both of these goals. This way, the cost and environmental impact criteria fit efficiently and effectively within the same MCDM mathematical model. Cost from the perspective of a customer is traced throughout the

product lifecycle by our model in a manner similar to that of the LCA treatment of the environmental impacts from the perspective of a stakeholder. The significance of data uncertainty is another commonality between the costs and environmental impacts. While the nature and level of these uncertainties may differ, each may be estimated by some probability function. Future work can focus upon finding the most accurate ways to represent the uncertainties. The work presented here considered the three-attribute model, focusing on the main impacts from nonrenewable resource consumption, environmental impacts, and cost over a product lifecycle. As such, the sub-attributes within nonrenewable resource consumption and environmental impact categories were grouped together. Future work can closely examine the comparison between the LCA grouping approach used here to simplify a design problem to a three-attribute HEIM model and the alternative of comparing all of the attributes within a larger HEIM model instead to consider the relative preferences among all attributes based on the type of product being designed. Such future work can also examine the effectiveness of the process to check for preference consistency within HEIM for each of these possible approaches.

In recent years, normative methods have proven successful for MCDM within the design process. Thus, the challenge to introduce MCDM at the conceptual design stages may be met by following a prescribed blueprint [7,8,,10,42,45]. Therein lies a solution to the identified challenge of implementing product design for sustainability at the conceptual design stages. This work shows that the normative method is equally applicable at the conceptual design stage when a baseline design is available for comparison. The work described in Chapter 7 builds on this work to identify the means to solve for the feasible preferred target point on the optimal design solution space. Moreover, our current study shows that as more specific design concepts are developed in greater detail, the application of engineering analysis or LCA could generate more accurate computations of each objective function in the design decision model. Thus, greater transparency of the environmental and economic impacts at each product lifecycle stage could improve understanding of the details of the effects by design engineers. Furthermore, adoption of

this method may coincide with the trend toward the further development over time of the LCI database and LCA methods toward increasingly greater comprehensiveness and accuracy. This chapter described the foundation methodology of NASDOP that was built upon by the work described in Chapter 7 to address many of these issues. NASDOP is a decision methodology for the sustainability-based design of products. The execution of such a decision generates information about its rationale and justification. Thus, an information model is needed to capture and communicate such information to all design participants. This topic is covered in the following chapter.

CHAPTER 6

IASDOP: AN INTEGRATED APPROACH TO INFORMATION MODELING FOR THE SUSTAINABLE DESIGN OF PRODUCTS

This chapter presents the published work³ by Eddy et al. [51]. Here, Design considerations are most effective when brought into a design process as early as possible, when design flexibility is normally greater in that the impact of any design change is mitigated. In their review, Ramani et al. [11] assert that early design considerations are even more important with the emergence of sustainable design. Sustainable product design can significantly affect the environment, economy, and societal well-being in a number of positive ways. In spite of the need, integration of sustainability considerations has progressed slowly. An ASME survey [552] supports the notion that design engineers are motivated to comply with current sustainability standards. The survey finds strongest sustainability interest among engineers to reduce energy and emissions. The survey also shows that organizations are most interested in compliance with regulatory requirements, and are most likely to only consider green methods that are cost competitive.

To support these current thrusts, this chapter proposes that sustainable design can be facilitated by introducing the guidelines provided by sustainability standards into early decision making criteria. The review by Ramani et al. [11] also identifies some challenges with the early design stage adoption of the needed sustainability considerations. Included among these considerations are support for decision making over an entire product lifecycle and modeling the information in an interoperable manner. To this end, this work explores the integration of guidelines for standards with the authors' earlier work in decision making for sustainability.

The prior chapter [46] introduced a normative decision analysis method for the sustainability-based design of products (NASDOP). NASDOP deploys (Life Cycle Assessment)

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LCA mathematical models with compatible (Life Cycle Costing) LCC models to consider both environmental and economic objectives during the evaluation of design alternatives. This work builds upon the prior work [46] in an important way. It provides a framework in which information pertaining to any applicable standards and regulations (henceforth only referred to as standards) is revealed transparently. Consequently, this information may influence the decision making process by highlighting criteria and constraints for consideration while also informing the decision maker during the articulation of preferences among the criteria considered.

A design process for sustainability often requires a comprehensive and holistic consideration of several distinct knowledge domains. Such an approach, if seamless, should improve upon the efficiency and effectiveness of a traditional design process that considers individual domains in a compartmentalized manner. However, integration of the major domains of a design process remains a topic of research. The work in this paper presents a novel approach to integrate the information models of four main domains to an extent not done in any known previous works. (Figure 5): Engineering Design, Sustainability Standards, Normative multi-criteria decision making, and LCA. The integration of all four of these domains will enable sharing of information in real time.

Section 6.2 details the key features of the new framework and its architecture. In Section 6.3, an illustrative case study is applied to demonstrate the framework's use in a design process. The final section discusses the results of this work. The next section summarizes prior works that have achieved some level of integration between two or more of the four domains of interest.

6.1. Related Works

First, this section looks at the relationship between LCA and other sustainability standards, indicators and metrics. An earlier approach established groups of key metrics represented within tools to serve as building blocks for the use of LCA [53], but it is not clear that the metrics used come from any established standards. More recently, a tool was developed to

combine site dependent data from LCA with environmental performance indicators to support decisions by aggregating output data into a comprehensible index [54]. A study to support considerations within an enterprise examined the use of LCA data aggregated into a performance index with that of other indicators and metrics, such as those related to compliance or eco-efficiency measures [55]. One of the more comprehensive descriptions of all such information pertaining to the multiple product sectors, and the relationships among standards, indicators, metrics, tools, and criteria, such as LCA criteria, is available at the website of the National Center for Manufacturing Sciences (NCMS) for Sustainability Project Initiative (SPI) projects [56]. Therefore, this work uses the content of this work to create a categorized library represented by the related information model described in the following section.

Prior work related to the modeling of sustainability metrics, standards, and indicators within ontological frameworks is also of interest. Yang and Song [57] constructed an ontological framework to represent LCA and LCC parameter inputs to use with criteria defined by sustainability metrics for the potential evaluation of alternatives within a design process for sustainability. A National Institute of Standards and Technology (NIST) workshop with industry [3] proposed that further harmonization and consolidation is needed between regulations, standards, and metrics. In response, researchers from NIST proposed use of the Zachman framework [58] to organize information from sustainability standards to facilitate modeling of the content within semantic frameworks such as ontologies. Such a means to organize the information is helpful due to the large number of standards and metrics and the redundancies and gaps between them. Researchers at NIST built upon this work by introducing a method to reason upon such information within an ontology to determine where such gaps and overlaps in sustainability standards exist [59]. With this methodology, overlaps can be found where similar concepts appear in different standards, and gaps reflect divergence of the concepts in different standards. Here, ontological information models of different standards are mapped to each other. This mapping process involves setting classes and properties equivalent to others whenever

possible. Such equivalencies are considered overlaps and the lack of equivalence was defined as a gap [59]. Reasoning may be done within the resulting ontology to determine which standards apply to specific products. Furthermore, an inconsistency of a specific product instance with a property value restriction imposed by the standards can indicate the lack of compliance of that product design.

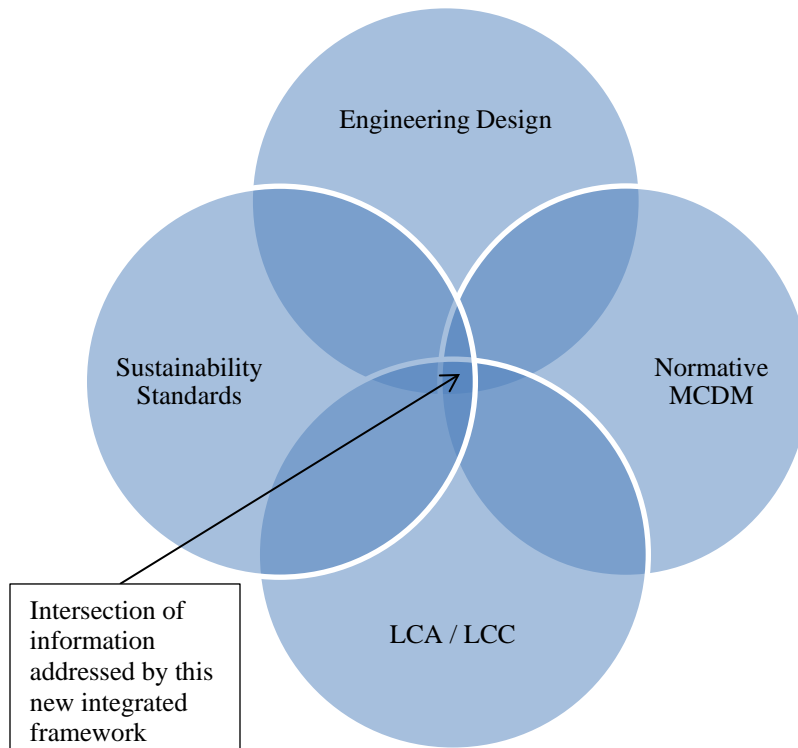


Figure 5: Desired state of information models for a design

Current literature [21,60-63] also emphasizes the importance of information modeling and its knowledge management pertaining to engineering design processes. The use of semantic web compatible ontologies has been shown to facilitate collaboration during distributed design and inform design decision making early in a design process, while also supporting interoperability of software tools deployed throughout the process. One such recent comprehensive review [60] highlighted the importance for the development of ontological

frameworks to capture design related knowledge in a flexible and robust manner and to also capture design rationale to support decision making early in a design process.

From a perspective of a design process for products, an ontological framework was constructed at the University of Massachusetts at Amherst to facilitate the documentation of design rationale for distributed design throughout an entire traditional design process [17-19,21]. As a result, the information is dynamically linked between the domains that comprise a design process. The hyperlinks of these ontologies may be imported for public use from [20] into software such as Protégé [65]. Future developments are planned to improve upon the visual format for sharing information by use of software such as OntoWiki [66]. Additional modules in the framework support the modeling of information for decision making with a Decision Support Ontology and with Decision Method Ontologies [16,67], which represent various methods to evaluate design alternatives having various attribute values.

The Decision Support Ontology and Decision Method Ontologies are aligned with the principles of Decision-Based Design, and as a result, can benefit a design process, especially when tradeoffs between conflicting objectives need to be considered for multi-criteria decision making. Decision-Based Design is based on some fundamental principles as defined by Hazelrigg [68]. Normative methods based on utility theory, which evaluate alternatives based on the maximization of utility, were developed for applications that require a certain degree of mathematical rigor [7,8,10,44]. One such method is hypothetical equivalents and inequivalents method (HEIM) [44,45], in which the optimal set of weights among multiple criteria is calculated based on the strength of preference expressed by a decision maker during the ranking of hypothetical alternatives. The resulting set of weights is used to compute the multi-attribute utility (MAU) value of any design alternative.

The integration between the domains of normative multi-criteria decision making and sustainable design has been limited despite the need. The often conflicting objectives of the triple bottom line for sustainability infer that multi-criteria decision making methods are well suited to

selecting optimal design solutions for sustainability. However, the introduction of usable normative methods to date has been limited. Thurston and her associates provided a constrained optimization methodology for sustainable product solutions [9,10]. More recently, HEIM was used to model the preferences of the decision maker in NASDOP [46]. Here, the uncertainties in the data from environmental emissions and costs were taken into account. For all of these reasons, the new ontological framework, introduced in this work, integrates the information used in this NASDOP methodology with this framework that includes the Decision Support Ontology and a Decision Method Ontology for HEIM.

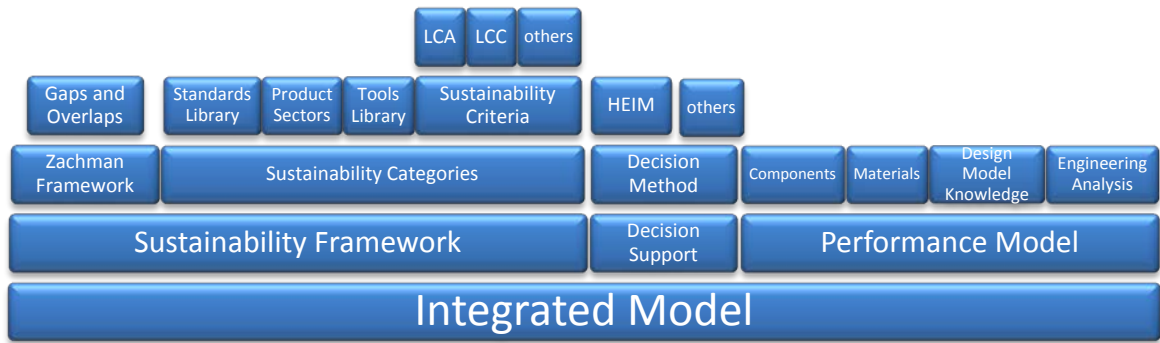


Figure 6: Modular building blocks of the information model for sustainable product design

The literature review, described in this section, alludes to the limited level of integration of information across domains in current design processes from the sustainability perspective. However, it can also be seen that these four main domains are all related to each other, and therefore, should not be modeled in isolation if the goal is to inform all participants in a design process. The work described in the next section provides such an integrated framework that dynamically links the information upon entry across these domains in a complete system.

6.2. IASDOP Architecture Framework

Here, the Integrated Approach for the Sustainable Design of Products (IASDOP) is described. Figure 6 illustrates the modular construction of the framework. The objects within

these domains are dynamically linked appropriately by the relationships between them as shown and described in the following sections. The ontology file is available to import and use from its webpage [69]. The following sections highlight some of the key features obtained by this construction.

6.2.1. Standard Fit within a Standards Library

Standard compliance has been identified as an important consideration in the design process for an enterprise [52]. The current process available to an enterprise to find a specific applicable requirement is inefficient at best due to the large number of standards and the corresponding missing and redundant information involved [3]. Selection of the appropriate standard depends greatly upon the product being designed. This suggests advantages with associations between standards and product sectors or the specific products within sectors. The Sustainable Standards Guide [56] highlights the content pertaining to the top level standards, product sectors, and also, criteria that may be used to measure sustainability objectives.

Figure 7 shows the upper level taxonomy comprised of the sustainability categories and the relationships linking these main categories of standards, products, and criteria. Relationships are shown graphically as arc types in these figures from within Protégé. Included in this taxonomy is a categorized library of sustainability standards without exhaustive detail of the information in each standard, which would likely change over time and require updating. This way, the specific standards applicable to a given product may be instantiated anytime a design instance is developed. There is also always a possibility that a current or potential standard applicable to a certain product does not have a standard within the library. Such circumstances are attended to in Section 6.2.3.

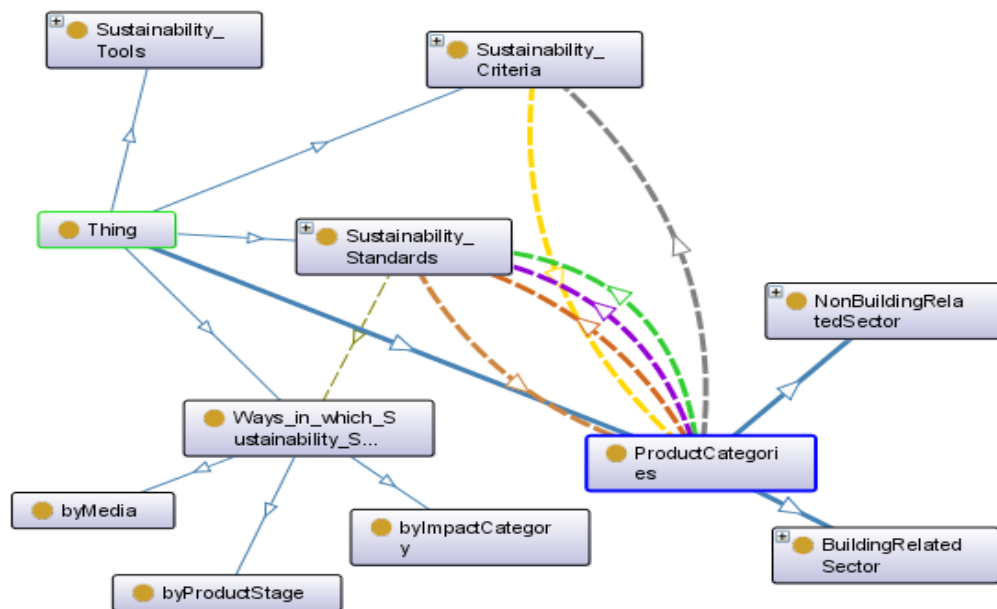
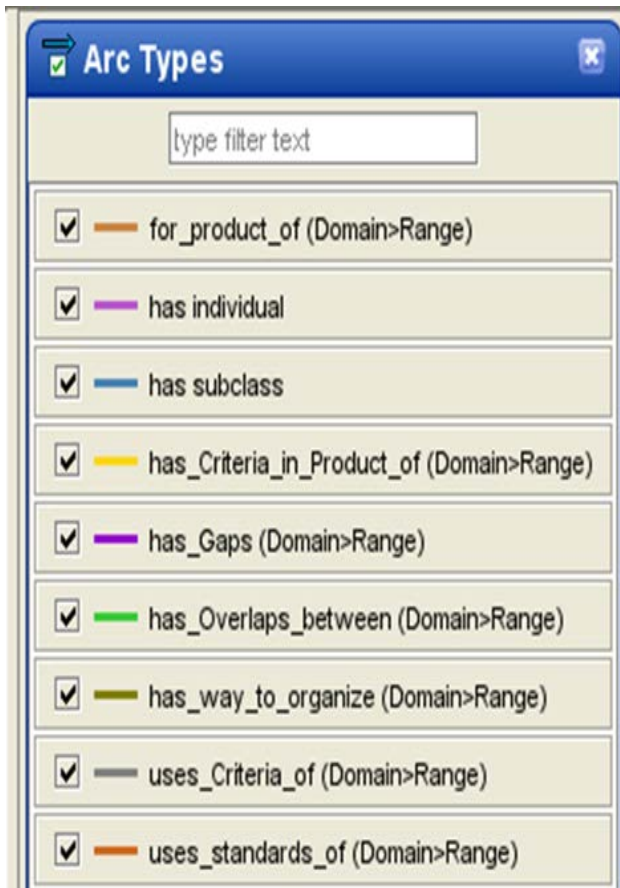


Figure 7: Relationships in the Sustainability Categories ontology

Arc Types

type filter text

- has individual
- has subclass
- hasCognitivePrimitive (Domain>Range)
- hasInformationAbstractionLevel(Subcla
- hasRole (Domain>Range)
- hasRole(Subclass all)



Figure 8: Relationships of the Zachman framework deployed

6.2.2. Relationships to the Zachman Framework

Standards can be complex and it can often be cumbersome to find the information sought. Researchers at NIST proposed use of the Zachman framework [58] to break down the information in a standard into an organized structure. To facilitate creation of the standards information models, this work deploys the prescribed ontological structure of the Zachman framework into an ontological framework module. Figure 8 shows such relationships of the prescribed matrix within the ontological framework. The class “Cells” consists of thirty-six possible categories, each corresponding to one of six different rows and columns. The top level relationships are also shown in Figure 8. Here, the top level row related to the context or objective scope of a standard is shown. Section 6.2.3 describes the key advantages that result from this ontological framework.

6.2.3. Revealing Gaps and Overlaps between Standards

The ontological framework can be especially useful for establishing dynamic relationships between standards and products to which they apply. Researchers at NIST suggest use of the relationships on the top context level of the Zachman framework to identify such gaps and overlaps [59]. The method to detect and model gaps and overlaps within an ontology may be deployed when all pertinent information is modeled in the ontologies for the standards being compared. Such an approach may be practical when a defined and limited scope of standards apply to the design endeavors of an enterprise. Here, this work aims to provide a generic framework that could be used in any design process. Thus, a library and information models more limited in their depth and scope of represented knowledge is used.

There are two different ways that such a generic framework can be used during a design process with potential effectiveness. Information models can be created for any applicable standards using the previously prescribed methods [58,59]. Alternatively, information may be entered as it is sought during a design process. Thus, this framework supports introducing the

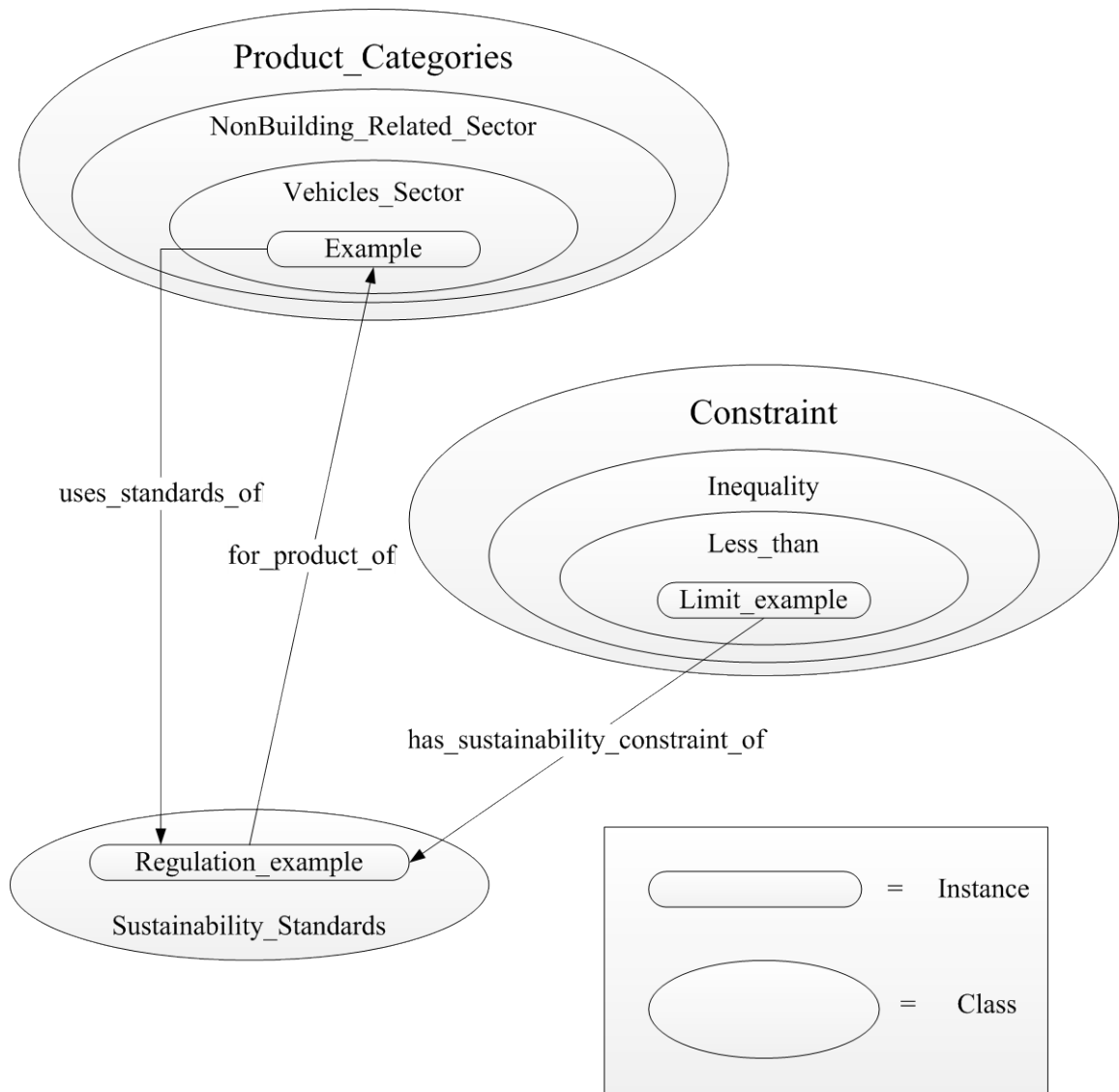


Figure 9: Relationships to constraints in a design process

guidelines and information provided by sustainability standards into a sustainable design process. This approach extends the definition of gaps introduced earlier [59] to include any requirement not yet specified in the existing standards library. Naturally, the depth of the standards' information models will determine the formalism and the extent of potential automation of these entries.

6.2.4. Revealing Constraints from Standards

From a design process perspective, an ultimate goal in modeling this knowledge which relates the standards and products is to define the applicable constraints for a given design situation. Survey information indicates that this is not usually a trivial task although rather important [3,52]. The diagram in Figure 9 shows an example of how such relationships may be established within this framework. Here, the constraints imposed by the standards are revealed for a product. Furthermore, these constraints are revealed in the engineering model along with other physical constraints related to the design. Thus, information models from standards inform the design model of any compliance related requirements. The example in Figure 5 depicts the case of a quantified regulatory limit. Depending upon the standard, some such constraints from standards may support mathematical modeling within constrained optimization programs, while others may be more qualitative and only applicable within information models.

6.2.5. The Integrated Framework

Other than the need to reveal the important constraints, a designer would also need to use this information within a decision model that reveals the rationale for selection of the most sustainable alternative. Here, other information models are integrated with those related to sustainability standards.

6.2.5.1. Three Information Models Combined

Figure 10 shows the class hierarchy of the taxonomy for sustainability criteria, which includes categories for LCA and LCC. Section 6.1 discussed some of the benefits of using multi-criteria decision making principles to design for sustainability. Efficiency and effectiveness of the early design stages should improve when all such criteria are considered together simultaneously in the same model rather than iteratively. To this end, ontological frameworks are integrated among sustainability, engineering design, and multi-criteria decision making (MCDM) domains.

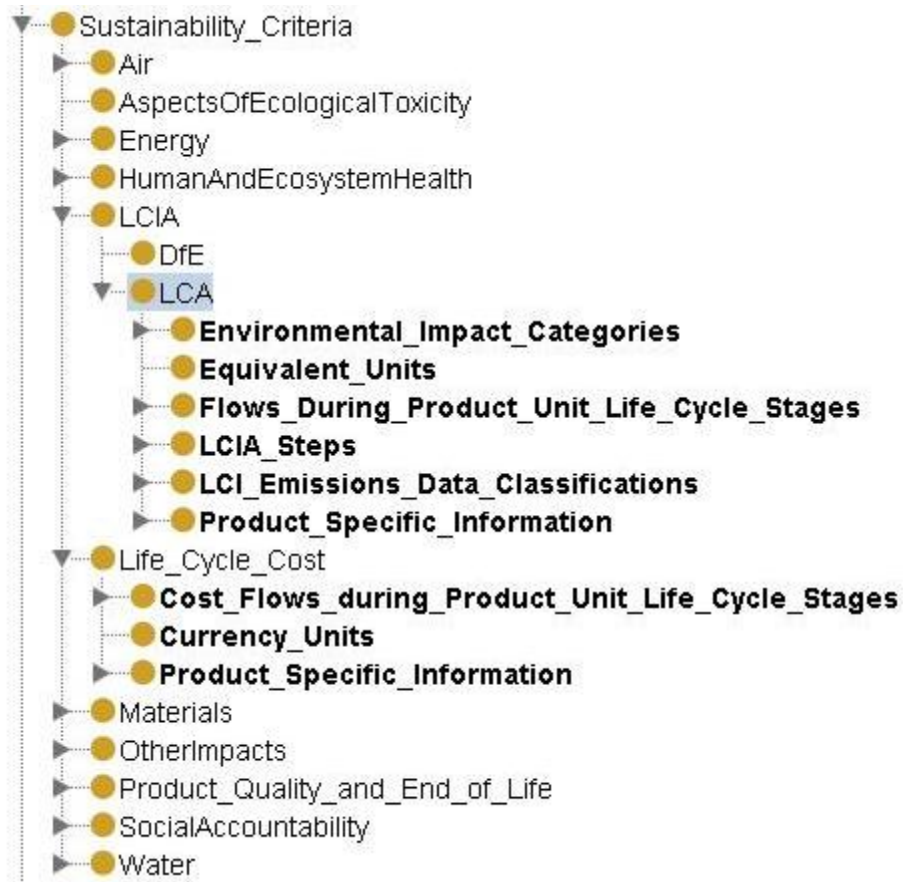


Figure 10: Criteria including LCA and LCC

Here, advantages are combined from an existing e-Design framework that captures and communicates information from a traditional design process [17], informs design model construction for decisions, and reveals decision rationale [16,67]. Such decisions should be made based on information pertaining to evaluation of the design option whose expectation has the highest value [68]. Such information can be defined concisely within the Decision Support Ontology combined with a given situation's most suitable Decision Method Ontology. Here, a Decision Method Ontology is introduced to represent the methodology for modeling the preferences among different criteria by using HEIM. HEIM has been implemented effectively in a sustainable design situation [46]. Furthermore, the units ontology from NASA [70] is integrated within this framework to verify that consistent units are used appropriately. Figure 11 shows the

mapping relationships between a design alternative instantiated in the Decision Support Ontology and the information in the new LCA ontology. The “has_working_solution” relationship in the Decision Support Ontology allows for the input of the information models of all criteria.

6.2.5.2. Products, Standards, and Criteria Relationships

Since each design situation will apply to a specific product, a design instance consists of a unique set of applicable criteria and standards. Figure 7 shows how this framework directly associates the relationships between a product and its standards and criteria. In doing so, information about the critical elements of the decision model is revealed transparently. Furthermore, this could aid the repository development of consolidated standards and criteria in the context of the products to which they are most applicable.

6.2.5.3. Common Ontology for Constraints and Criteria

Constrained design optimization methods provide the means to consider criteria and constraints simultaneously. The approach of this work advocates modeling information from standard requirements as constraints. Even in cases when such requirements cannot be expressed in the same mathematical model for optimization, the information model can reveal such constraints transparently to alert designers of the need for compliance verification by deployment of the semantic reasoning method [59] described in Section 6.1. Section 6.1 also points out that in spite of the need to combine sustainability standards with objectives such as the minimization of environmental impacts; such prior work has been very limited.

In recent years, LCA has evolved into a prescribed method to measure value in terms of environmental impacts. LCA determines impact criteria based on standards of ISO 14040-14044, TRACI , and others. A number of different LCA methods were developed to characterize, group, normalize, and weight the impacts for assessment. This framework uses the EDIP 2003 method

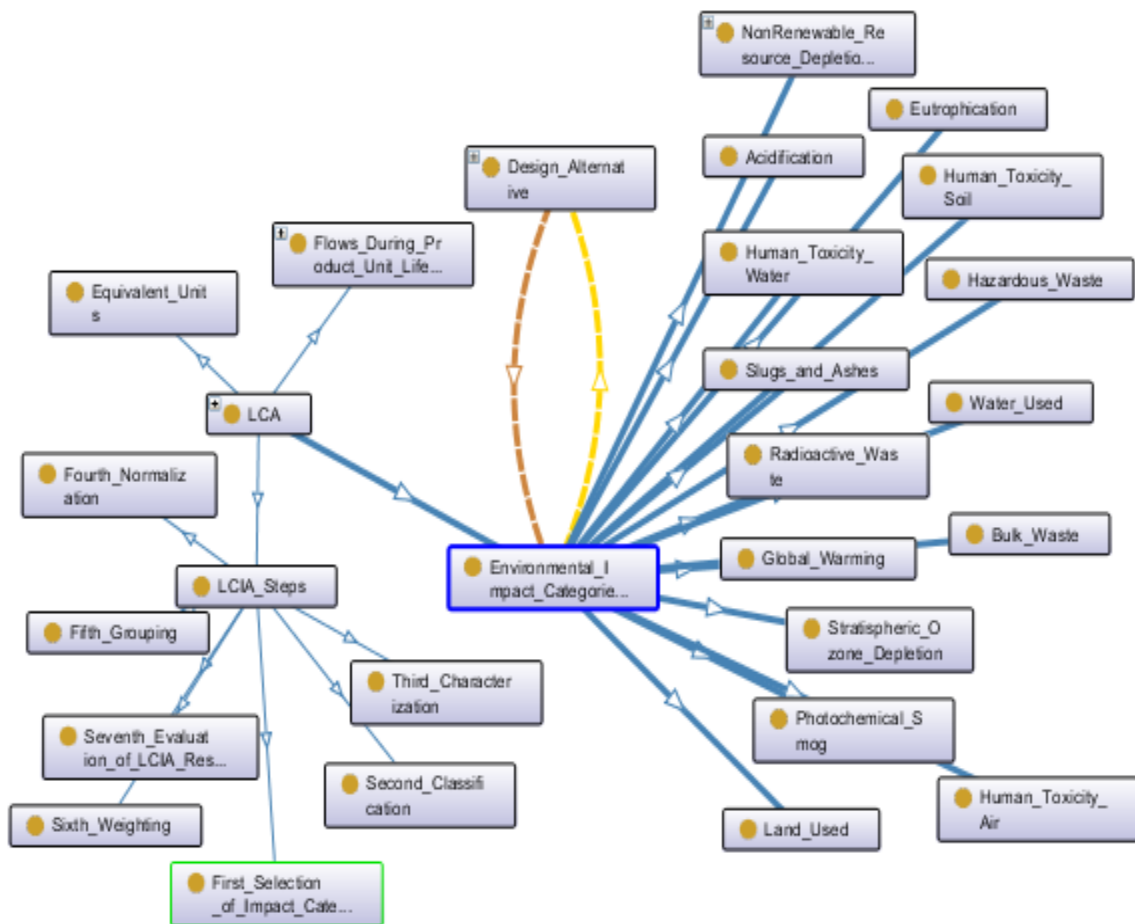
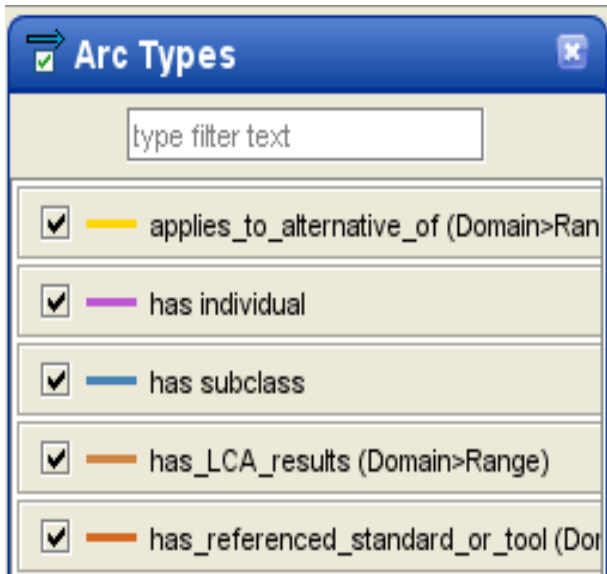


Figure 11: LCA module construction

within SimaPro for consistency with the NASDOP methodology that was developed to deploy multi-criteria decision making for sustainable product design [46]. Relationships between modules in the framework provide the connection of resulting environmental impact information to information about the evaluation of design alternatives that inform the decision making process in the Decision Support Ontology. Figure 11 shows the representation framework for established LCA methodology. The context of criteria shown in Figure 10 indicates that multiple criteria related to sustainability could be involved in a model.

6.2.6. The Integrated Design Process

Due to the integration of the framework, the rationale of the design situation and the applicable standards combine to inform the pertinent optimization model. From there, the optimal design alternative can be identified in parallel with the inspection of compliance to any applicable standards. Since every product design is different, this IASDOP framework is constructed with the flexibility to accommodate a wide array of design situations. The following section describes the use of the fully integrated IASDOP framework and the enabled design process in one such actual design case study. This case study illustrates how these presented advantages of IASDOP specifically contribute to a successful design.

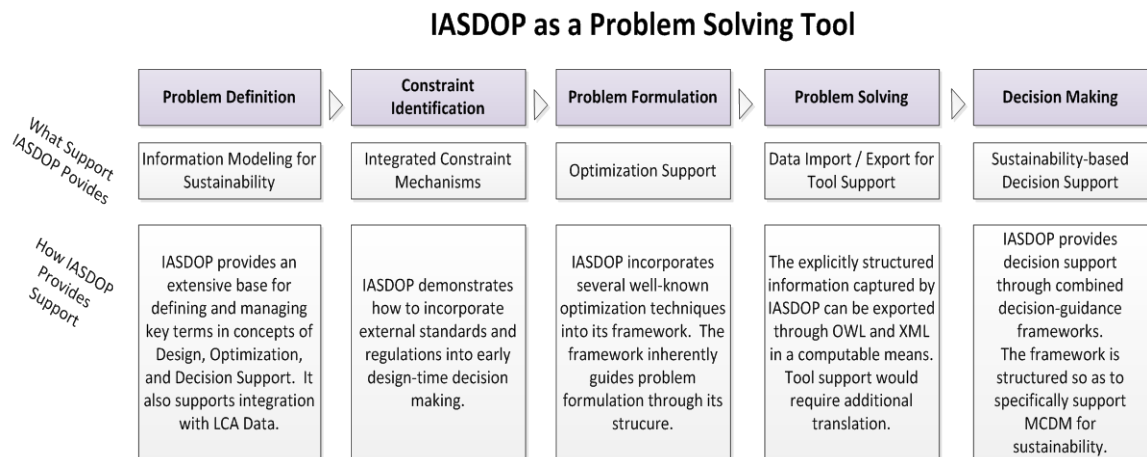


Figure 12: Specific contributions of IASDOP to a successful design process for sustainability

6.3. CASE STUDY: Sustainability of Brake Disk Rotor and Pads

This case study has been divided into five sections. Figure 12 shows the specific contributions corresponding to Sections 6.3.2 thru 6.3.6. This outline specifies and illustrates improvements to a design process by the support of sustainability considerations.

6.3.1. Brake Disk Rotor and Pads

This case study uses IASDOP to capture and communicate information about the utility evaluation for the optimal set of automotive brake disk rotor and companion pair of caliper pads. In this case, it is assumed that a five year life of these parts is desired along with other assumptions reasonable for a typical midsize passenger automobile. Mathematical models were constructed based on conventional engineering formulations [71] to estimate results. Here, it is assumed that consumers desire the performance objective of minimizing the vehicle stopping distance subject to the performance constraints of adequate heat dissipation, a temperature limited to less than 77 degrees C, and adequate rotor and pad thickness remaining at the end of five years of typical use.

6.3.2. Problem Definition: Information Modeling for Sustainability

Some research provides engineering data for the most common rotor materials [72], and more general information is available regarding caliper pad material options. Thus, each possible material combination may reasonably represent a design alternative. Independent variables consist of the geometry of the parts, which in this case is limited to the initial thickness of the rotor and pads and the percentage of the rotor that is solid. Most rotors have hollowed fins to increase convective cooling. Other than material type, the weight of the parts is the most significant factor for the minimization of the impacts given by both LCA and LCC. Stopping distance was found to be independent of weight and geometry whenever all performance constraints are satisfied. These performance constraints, such as assuring that the brake materials

dissipate heat quickly enough and do not wear too thin during the product life, are different from constraints imposed by sustainability standards, which will be explained shortly. In the interest of optimizing for sustainability considerations, the weight for each material combination alternative was optimized. Here, the optimal geometry of the parts was determined for each alternative. Models to generate solutions were developed within Parametric Technology Corporation's MathCAD software [73]. Optimization capabilities of Phoenix Integration's ModelCenter software [74] with their MathCAD plugin were deployed to optimize the mass for each design alternative subject to the performance constraints.

LCA results were estimated using SimaPro software [75] based on some reasonable assumptions given the data available for each of the common material combinations. LCC was estimated from available generic searches for cost data. The information mentioned here was modeled appropriately in the IASDOP framework. Section 6.1 discussed the need to satisfy the triple bottom line multiple objectives for sustainability of preserving the environment, the economy, and the interests of the stakeholders in society. Thus, optimization was done among the three main objectives of minimization of vehicle stopping distance, as well as the minimization of environmental and cost impacts over the product's life cycle. Table 9 highlights the information model created to represent these three main objectives and their associated variables.

6.3.3. Constraint Identification: Integrated Constraint Mechanisms

The first step involved a search to find the specific standards and regulations that apply to the design situation. A general web search for those applicable to this product design reveals three potentially consequential regulations, which all pertain to material selection in this design process. Brake caliper pads were often made from asbestos material in the past, later raising human health and safety concerns [76]. Related standards were documented as instances within the framework of categorized standards. It is also possible for a standard of concern to not yet be modeled in the framework. Standards may be most applicable to certain product groups, such as

limits on copper content to 0.5 % in these brake disk parts due to concerns about the cause of some toxic substances in water. The application of some standards to a certain product may require more investigation. For example, disk brakes emit dust during operation, and silica

Table 9: Main design criteria and their independent variables

Subject Instance in "Objective_Function" Class	Relationship in "Objective_Function" Class	Object Instance or Value
Comparative_cost	goal	minimize
	used_in_model	Brake_disk_and_pad_performance
	has_unit	Currency_units_USD
	has_objective_parameter	Variable_massPercentDisk
		Variable_tDisk
		Variable_tPad
considered_in	evaluation_to_Maximize_MAU_utility_value	
Greatest_environmental_impact	goal	minimize
	used_in_model	Brake_disk_and_pad_performance
	has_unit	Equivalent_units_Pt
	has_objective_parameter	Variable_massPercentDisk
		Variable_tDisk
		Variable_tPad
considered_in	evaluation_to_Maximize_MAU_utility_value	
Stop_distance	goal	minimize
	used_in_model	Brake_disk_and_pad_performance
	has_unit	meter
	has_objective_parameter	Variable_massPercentDisk
		Variable_tDisk
		Variable_tPad
considered_in	evaluation_to_Maximize_MAU_utility_value	
Minimize_weight	goal	minimize
	used_in_model	Brake_disk_and_pad_performance
	has_unit	kilogram
	has_objective_parameter	Variable_massPercentDisk
		Variable_tDisk
		Variable_tPad
considered_in	evaluation_to_Maximize_MAU_utility_value	

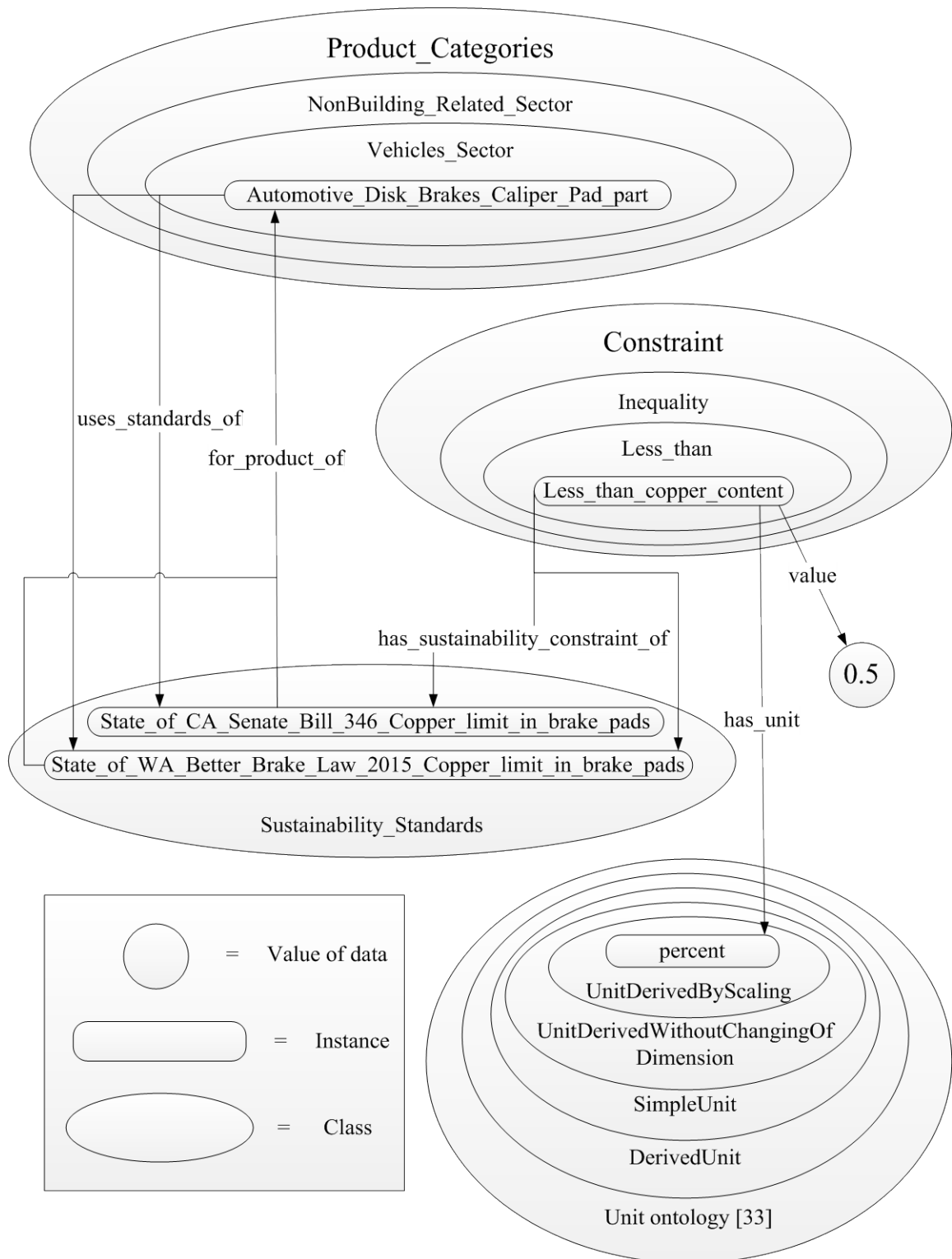


Figure 13: Modeling of a constraint imposed by sustainability standards

dust concentrations are limited for health reasons [77]. These various standards were modeled in relation to the design instance of this specific product within the integrated framework. This was accomplished by the use of the framework as described in Sections 6.2.1 to 6.2.5. Figure 13 shows the constraint imposed by the sustainability standards related to copper content in a common engineering design model. Thus, sustainability standards are informing the design model as Section 6.2.4 emphasizes.

6.3.4. Problem Formulation: Optimization Support

The framework allows modeling of sustainability standards and criteria within a shared configuration. Any relationships between standards and criteria can extend to modeling of design information in that constraints can influence design criteria. Furthermore, constraints and criteria can potentially be modeled in the same design optimization formulation if they can be expressed as mathematical functions with the same independent variables. Current standards usually are not expressed in such a mathematical format. However, such sustainability constraints and criteria may be included in the same information model as highlighted in prior figures and sections.

Section 6.2.5 highlights the integration of information models for sustainability, engineering design, and multi-criteria decision making. Use of this framework initially to identify the standards and regulations transparently can lead to identification of criteria related to minimization of critical environmental impacts. This is done by using the ontological module for LCA, which is built into the sustainability criteria category of the framework. Figure 14 shows this case study within the LCA module of the framework.

6.3.5. Problem Solving: Data Import / Export for Tool Support

This case study illustrates that this decision making process, which is outlined in Figure 12, of selecting the optimal design alternative combines several considerations simultaneously. The information is integrated among the four domains shown back in Figure 5 by dynamically

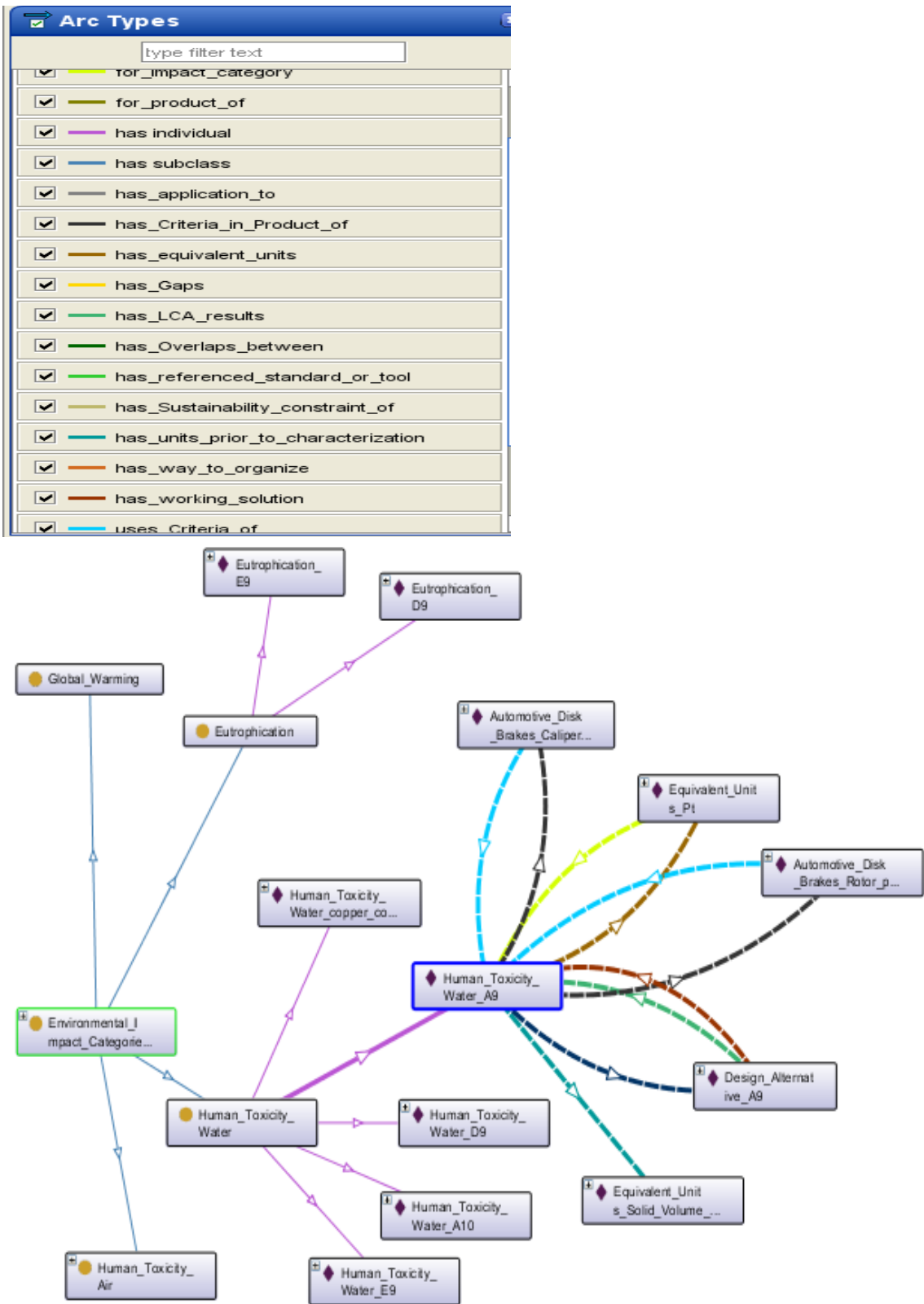


Figure 14: Use of information from LCA to compare impact results among alternatives

Properties of frmk:Design_Alternative_A9	
dso:abstraction_level	mixed
dso:has_design_summary	<ul style="list-style-type: none"> ▣ frmk:Feature_Pad_thickness_A9 ▣ frmk:Feature_Rotor_thickness_A9 ▣ frmk:Feature_rotor_mass_fraction_A9 ▣ frmk:Iron_Grey_Cast ▣ frmk:Steel_stock
dso:has_working_solution	<ul style="list-style-type: none"> ▣ frmk:Cost_Flows_during_Product_Unit_Life_Cycle_Stages_A9 ▣ frmk:Human_Toxicity_Water_A9 ▣ frmk:Model_Performance_for_A9
dso:is_alternative_for	<ul style="list-style-type: none"> ▣ frmk:issue_product_Select_Brake_disk_material_combination
frmk:has MAU value	0.956
frmk:has_objective_function_value_f1	144.6
frmk:has_objective_function_value_f2	0.024
frmk:has_objective_function_value_f3	15.34
frmk:has_utility_value_u1	0.926
frmk:has_utility_value_u2	0.956
frmk:has_utility_value_u3	0.972
inta:has_LCA_results	<ul style="list-style-type: none"> ▣ frmk:Human_Toxicity_Water_A9
rdf:type	<ul style="list-style-type: none"> ▣ dso:Design_Alternative
rdfs:comment	This considers the design option of a grey cast iron rotor and steel caliper pads.

Geometry related

Material related

Best alternative with the highest MAU value

Properties of frmk:Human_Toxicity_Water_A9	
frmk:Copper_main_emissions_to	Water
frmk:Silicon main emissions to	Water
frmk:emits_total_grams_of_copper	49.3
frmk:emits_total_grams_of_silicon	351.0
inta:applies_to_alternative_of	<ul style="list-style-type: none"> ▣ frmk:Design_Alternative_A9
lca:has_characterization_factor_value_of	2.76E-5
lca:has_equivalent_units	<ul style="list-style-type: none"> ▣ frmk:Equivalent_Units_Pt
lca:has_units_prior_to_characterization	<ul style="list-style-type: none"> ▣ lca:Equivalent_Units_Solid_Volume_cu_meter
lca:has_value_sum_of_all_five_life_cycle_stages	0.024
sstc:has_Criteria_in_Product_of	<ul style="list-style-type: none"> ▣ frmk:Automotive_Disk_Brakes_Caliper_Pad_part ▣ frmk:Automotive_Disk_Brakes_Rotor_part
rdf:type	<ul style="list-style-type: none"> ▣ lca:Human_Toxicity_Water
rdfs:comment	Critical environmental impact for the design option of a grey cast iron rotor and steel caliper pads.

Copper content during the product lifecycle

Greatest environmental impact of this alternative in Pt units

Figure 15: Results of the most preferred design alternative – baseline for comparison

Properties of frmk:Design_Alternative_A10

dso:abstraction_level	mixed
dso:has_design_summary	<ul style="list-style-type: none"> ▣ frmk:Composite_Copper_fibers ▣ frmk:Iron_Grey_Cast
dso:has_working_solution	<ul style="list-style-type: none"> ▣ frmk:Cost_Flows_during_Product_Unit_Life_Cycle_Stages_A10 ▣ frmk:Human_Toxicity_Water_A10 ▣ frmk:Model_Performance_for_A10
dso:is_alternative_for	<ul style="list-style-type: none"> ▣ frmk:issue_product_Select_Brake_disk_material_combination
frmk:has_MAU_value	0.854
frmk:has_objective_function_value_f1	158.5
frmk:has_objective_function_value_f2	0.0497
frmk:has_objective_function_value_f3	14.05
frmk:has_utility_value_u1	0.563
frmk:has_utility_value_u2	0.879
frmk:has_utility_value_u3	0.978
inta:has_LCA_results	<ul style="list-style-type: none"> ▣ frmk:Human_Toxicity_Water_A10
rdf:type	<ul style="list-style-type: none"> ▣ dso:Design_Alternative
rdfs:comment	This considers the design option of a grey cast iron rotor and coper fiber caliper pads.

MAU value decreased from baseline

Properties of frmk:Human_Toxicity_Water_A10

frmk:Copper_main_emissions_to	Water
frmk:Silicon_main_emissions_to	Water
frmk:emits_total_grams_of_copper	140.3
frmk:emits_total_grams_of_silicon	81.4
inta:applies_to_alternative_of	<ul style="list-style-type: none"> ▣ frmk:Design_Alternative_A10
lca:has_characterization_factor_value_of	2.76E-5
lca:has_equivalent_units	<ul style="list-style-type: none"> ▣ frmk:Equivalent_Units_Pt
lca:has_units_prior_to_characterization	<ul style="list-style-type: none"> ▣ lca:Equivalent_Units_Solid_Volume_cu_meter
lca:has_value_sum_of_all_five_life_cycle_stages	0.0497
sstc:has_Criteria_in_Product_of	<ul style="list-style-type: none"> ▣ frmk:Automotive_Disk_Brakes_Caliper_Pad_part ▣ frmk:Automotive_Disk_Brakes_Rotor_part
rdf:type	<ul style="list-style-type: none"> ▣ lca:Human_Toxicity_Water
rdfs:comment	Critical environmental impact for the design option of a grey cast iron rotor and coper fiber caliper pads.

Copper content increased by a factor of 2.85 from baseline

Environmental impact increased by a factor of 2.07 from baseline

Figure 16: Results of an alternative with some copper content in the caliper pads

Properties of frmk:Design_Alternative_E9	
dso:abstraction_level	mixed
dso:has_design_summary	<ul style="list-style-type: none"> ▣ frmk:Composite_0.20_SiC_reinforced_Al-Cu_alloy_AMC_2 ▣ frmk:Steel_stock
dso:has_working_solution	<ul style="list-style-type: none"> ▣ frmk:Cost_Flows_during_Product_Unit_Life_Cycle_Stages_E9 ▣ frmk:Eutrophication_E9 ▣ frmk:Model_Performance_for_E9
dso:is_alternative_for	<ul style="list-style-type: none"> ▣ frmk:issue_product_Select_Brake_disk_material_combination
frmk:has MAU value	0.631
frmk:has_objective_function_value_f1	142.2
frmk:has_objective_function_value_f2	0.229
frmk:has_objective_function_value_f3	36.88
frmk:has_utility_value_u1	1.0
frmk:has_utility_value_u2	0.112
frmk:has_utility_value_u3	0.879
inta:has_LCA_results	<ul style="list-style-type: none"> ▣ frmk:Eutrophication_E9 ▣ frmk:Human_Toxicity_Air_E9 ▣ frmk:Human_Toxicity_Water_E9
rdf:type	▣ dso:Design_Alternative
rdfs:comment	This considers the design option of a 20% SiC reinforced Al-Cu alloy (AMC 2) rotor and steel caliper pads.

MAU value decreased more from baseline

Properties of frmk:Human_Toxicity_Water_E9	
frmk:Copper_main_emissions_to	Water
frmk:Silicon_main_emissions_to	Water
frmk:emits_total_grams_of_copper	497.1
frmk:emits_total_grams_of_silicon	1370.0
inta:applies_to_alternative_of	▣ frmk:Design_Alternative_E9
lca:has_characterization_factor_value_of	2.76E-5
lca:has_equivalent_units	▣ frmk:Equivalent_Units_Pt
lca:has_units_prior_to_characterization	▣ lca:Equivalent_Units_Solid_Volume_cu_meter
lca:has value sum of all five life cycle stages	0.171
sstc:has_Criteria_in_Product_of	<ul style="list-style-type: none"> ▣ frmk:Automotive_Disk_Brakes_Caliper_Pad_part ▣ frmk:Automotive_Disk_Brakes_Rotor_part
rdf:type	▣ lca:Human_Toxicity_Water
rdfs:comment	Secondary environmental impact for the design option of a 20% SiC reinforced Al-Cu alloy (AMC 2) rotor and steel caliper pads

Copper content increased by a factor of 10.1 from baseline

Environmental impact increased by a factor of 7.13 from baseline

Figure 17: Results of an alternative with increased content of both copper and silicon in the rotor

linking information across domains by the relationships set up in the ontological framework. Not only is this study looking at three different attributes in multi-criteria decision making, but it also reveals three different standards or regulations that should be met. It is assumed that caliper pads made from asbestos should not be considered due to the obvious health risks. The information in this model reveals that rationale. The means to comply with the standards that limit copper and silica content is not quite so obvious. Since LCA is assessed for each material combination alternative anyways, perhaps that information can help.

Figures 15-17 illustrate this by showing the specific results for both LCA and multi-criteria decision making side by side for three of the alternatives. The instantiated ontology is shown from OntoWiki software [66] in these three figures. Figure 15 represents the results of the best feasible choice, which was evaluated to have the highest multi-attribute utility (MAU) value. Here, instance locations of the optimal design geometry and material are shown and specifics would be revealed by simply double clicking on such desired instance links in the ontology. SimaPro generates estimates of all the main environmental impact groups, but usually one specific impact exceeds all the others. For this alternative, human toxicity in water content has the greatest impact. This material combination is a grey cast iron rotor with steel caliper pads. Assumptions are made during LCA and LCC, because the data is not always available for the exact materials and processes involved in the life cycle of every product design. Regular cast iron and steel materials may have less impact and cost than many other materials that may require more processing during the material extraction. This best choice is based on the preferences expressed in the HEIM information model. Use of the integrated framework allows dynamic linking of the information across the domains.

6.3.6. Decision Making: Sustainability-based Decision Support

The inventory of copper and silicon emitted during the life cycle can also be inspected. Most of the emitted mass in these instances flows to the water rather than the air or soil. Thus, the

standard for copper is more likely to apply than the standard for silica dust in the air in this case. Figures 15-17 also show the emissions to water of copper and silicon for the three alternatives illustrated. Figure 16 shows results for a grey cast iron rotor and a copper fiber composite caliper pad material. The copper fiber material is not likely to meet the standard for sale in the states of California or Washington. It is interesting that the standard is based on the copper mass percentage of the material, but the information shown regarding the copper emissions to water may actually be more reflective of the impacts of concern. Either way, it is evident that both the human toxicity in water and the copper emissions to water are both nearly doubled or tripled when the alternative changes to the copper fiber material for the pads. Figure 17 assesses a rotor made from a 20 % SiC reinforced Al-Cu alloy (AMC 2) instead of the grey cast iron rotor shown in Figure 15. As a result, eutrophication of the water exceeds the human toxicity in the water as the most significant impact, and the impact approaches ten times more significant. It is interesting that the copper emissions to the water are also about ten times greater. Thus, there is some consistent correlation between the standards and the LCA criteria in this case. This shows that some understanding of relationships between standards and critical impacts can be gained early in a design process by the use of this framework. The resulting multi-attribute utility (MAU) values shown in Figures 15-17 reveal the rank of these alternatives from best to worst.

6.4. Discussion of Results for IASDOP

The main objective of this work was to support informed design decisions for sustainable product design objectives through the early integration of sustainability standards and criteria. A successful result will ease the adoption of the pertinent standards and regulations and also influence a design toward the objectives related to sustainability. This work integrated information models from the four domains shown in Figure 5 to demonstrate how such integration can benefit a design process for sustainability.

In traditional engineering design, requirements introduce constraints, which can influence criteria. Design involves a decision, among alternatives, that best satisfies the criteria, which define the issues. The decision may introduce more or new constraints for subsequent design iterations. A design process generates information, which can best be represented by information models accessible by all design participants. The findings in this work support the use of such established principles for sustainability considerations.

Furthermore, the case examined shows that some consistencies can be revealed between applicable regulations modeled by standards and environmental impacts determined by LCA. The process enabled by the IASDOP framework was shown to allow parallel inspection of information related to standards and design alternative selection. This work began with the premise that sustainability standards and regulations may be aligned with the triple bottom line objectives of sustainability. Although this may or may not be true depending upon the standard, a framework is provided in which the information is connected by the relationships. This connection should be evident in all cases. Although compliance with standards and regulations could require further validation, the intent shown in the information about the standards does have some alignment with the triple bottom line criteria in the case observed. Thus, efficiency and effectiveness may be improved by the use of this framework in many other cases as well. Since instantiation of the design information does involve some time and resources, design teams should evaluate the expected cost and benefits of using this method on a case by case basis. An additional benefit of the instantiation could be realized by the capability to query the information based on its context and meaning. Future work may investigate possible use of the reasoning and rules capabilities of the ontologies to identify any further potential to improve decision making.

Any such method becomes much more useful when the benefits can be realized as early in a design process as possible. The case presented here shows one example in which a sustainable design may depend exclusively upon the independent variables of the material and geometry of the components for their given use. Thus, the method deployed could be

implemented at the early stages of conceptual design in some cases. The following chapter looks at full design space exploration that may involve response surface modeling from known data and the construction of surrogate models. The successful construction of reliable solution models that depend exclusively upon the geometry and material of the components should significantly aid the adoption of the methodology as early in a design process as possible.

CHAPTER 7

MASSDOP: A ROBUST SURROGATE MODELING APPROACH FOR MATERIAL SELECTION IN SUSTAINABLE DESIGN OF PRODUCTS

The selection of the optimal material, while considering objectives for sustainable design comprehensively early in a design process, can significantly improve the overall impacts of products⁴. Ljungberg argued that material selection is one of the most important factors that affect the quest to achieve more sustainable products [79]. 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 [80]. Other researchers found LCA, in its current form, to be unsuitable for use by designers at the early stages of a product design [81]. A recent review paper [11] and the recent National Institute of Standards and Technology (NIST) workshop on sustainability [3] 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 [82,83].

However, very few implementations exist of surrogate model solutions for sustainable product design. Even more surprising is the lack of prescribed metamodeling techniques for optimal material selection for engineering problems in general. A surrogate model may also be referred to as a response model or metamodel, or a model of a model, that substitutes for another high fidelity, physics-based model by merely interpolating discrete input and output points of data to statistically approximate the input output function experimentally independent of the underlying physical laws [84]. Hazelrigg [85] distinguishes between descriptive and predictive models for engineering design, and advocates for the use of predictive models during early design

⁴ Public access is conditional upon pending permission to reprint by the potential publisher as of the time of this writing (American Society of Mechanical Engineers). Access of this dissertation was made conditional upon reprint permission being granted after paper [78] publication by ASME.

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 modeling error, should be used where more precise representations are needed of the physical system behavior for more detailed engineering analysis.

The use of metamodels for sustainable design remains a topic of research. Zhou et al. [86] proposed a notable possible approach to address both of the research gaps of a lack of surrogate modeling techniques for sustainable design and the lack of such techniques for optimal material selection. Their method integrates artificial neural networks (ANN) with genetic algorithms (GAs) for optimal material selection in consideration of mechanical, economic, and environmental properties. Sousa et al. [87] developed an ANN surrogate modeling method to better streamline the LCA process and define some product groupings. More recently, Sousa and Wallace [88] used these groupings to develop a product classification system by deployment of learning surrogate models constructed from the groupings.

This chapter advocates use of the mathematical rigor of a normative approach for sustainable design. Hazelrigg [89] also asserts that a model needs to find local optimal designs and also determine which of the local neighborhoods 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 [46]. 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, etc. Material selection becomes more important when sustainability is considered. The challenges in this area were exposed in prior work. Rydh and Sun [90] 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 the impact attributes during various life cycle stages. 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, the following sections introduce such a novel approach and a new methodology for a robust surrogate modeling approach for material selection in sustainable design of products (MASSDOP). The next section discusses important issues related to a product's life cycle. Section 7.2 prescribes a fundamental foundation to formulate a problem by representing the entire design space. Section 7.3 introduces a mapping methodology for modeling. Section 7.4 provides novel surrogate model construction and testing techniques for material selection. Section 7.5 addresses issues related to optimization of a constructed surrogate model. Section 7.6 demonstrates how the entire methodology can be used with a case study example of the design of a disc brake for an automobile. Section 7.7 discusses the results in the context of the challenges that this work aims to address.

7.1. The Product Life Cycle

The fundamental first step is to identify the significant life cycle processes that must be considered. A holistic approach to design for sustainability needs to consider all attributes over the complete life cycle of the product. However, the significance of the effects at various life cycle stages indicates that various product life stages should be considered at the most appropriate time in a design process. For example, the intended use of a product should be considered at the earliest design stages. Aside from any major localization issues, decisions regarding the mode of

distribution of the product and its components throughout the supply chain may often be best to decide later in a design process. The following subsections address the most appropriate design stages to consider the costs and environmental impacts from each of the five main product life cycle stages. These five main stages include materials extraction, components and product manufacturing, product distribution, product use, and end of life disposition of the product and its components.

7.1.1. Product use stage issues

Identification of the functional use of a product could have the most significant effect on the resulting performance, cost, and environmental impacts. Such alternatives should be carefully considered during the early design stages, which offer the greatest design flexibility. To this end, prior published approaches [34,91] provide the means to map various functions and associated forms to associated environmental impacts. However, such approaches have limited accuracy to which the environmental impacts can be determined. Other work [92] focuses on the abstract relationships of affordances, rather than functions, to environmental impacts.

This paper 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. This approach should complement the prior approaches and round out the suite of methods available to engineers comprehensively. Once one can presume that all design alternatives in a design space have the same prescribed general form and function, impacts during the product use life cycle stage reduce to any differences such as more or less energy consumed due to different mass, inertia, thermal conductivity, etc., or more or less consumable parts used per year [87]. The significance of such differences would be problem specific. The next subsection discusses the remaining life cycle stages of material extraction, manufacturing, and end of life disposition. A more general approach could be applicable to these three product life cycle stages.

7.1.2. Identification of significance for early design efficiency

The early stages of conceptual design can benefit from approximation models and methods that efficiently identify the optimal concept to proceed with. To this end, the approach described by this paper focuses on the most significant and the least complex contributions to environmental impacts. All life cycle stages can be modeled by using the Life Cycle Assessment (LCA) process [28,29]. Software tools such as SimaPro [30] or GaBi [93] automate the computational mapping of any life cycle processes to the resulting environmental impacts. Such impacts are grouped categorically, normalized to have equivalent units of Ecopoints [Pt], and weighted based on severity to sum together in a single equation all using one of several viable methods [94].

Processes related to the initial stage of material extraction and the final stage of end of life disposition of product components may be entered on a simple mass unit basis. The work presented in this paper includes the LCA modeling of all processes involved in the production and end of life disposition of one kilogram of seventy-eight different materials for which the pertinent information and data exists. Thus, a design set of alternatives can reduce to selection from among various material choices and their associated weights or volumes. The manufacturing life cycle stage is also an important stage to consider. The key question becomes when the appropriate time in the design process to consider such impacts is.

7.1.2.1. Appropriate design stage to consider manufacturing impacts

The key point to consider is whether or not consideration of manufacturing impacts is likely to have a significant effect on which material alternative is most optimal. The graph in Figure 18 shows, by an example of the case of machining steel or aluminum to half its mass, that the processes related to material acquisition and disposal are generally much more significant to environmental impacts than are those due to such a manufacturing process. This does not mean

that impacts during manufacturing are not significant, because they indeed are. However, the results shown in Figure 18 indicate that they are not nearly as likely to affect the material selected as the material type itself would. Identification of the manufacturing process alternatives can be relatively complex. Furthermore, modeling of all manufacturing processes alternatives for every material alternative in LCA computational models can be time consuming. However, differences in cost among alternatives can be more significant than environmental impact differences during the manufacturing stage. Many organizations have developed their own efficient and reliable cost estimation standards to facilitate concept selection during the early design stages. Here, more established Design for Manufacturability (DFM) approaches [95] can be used.

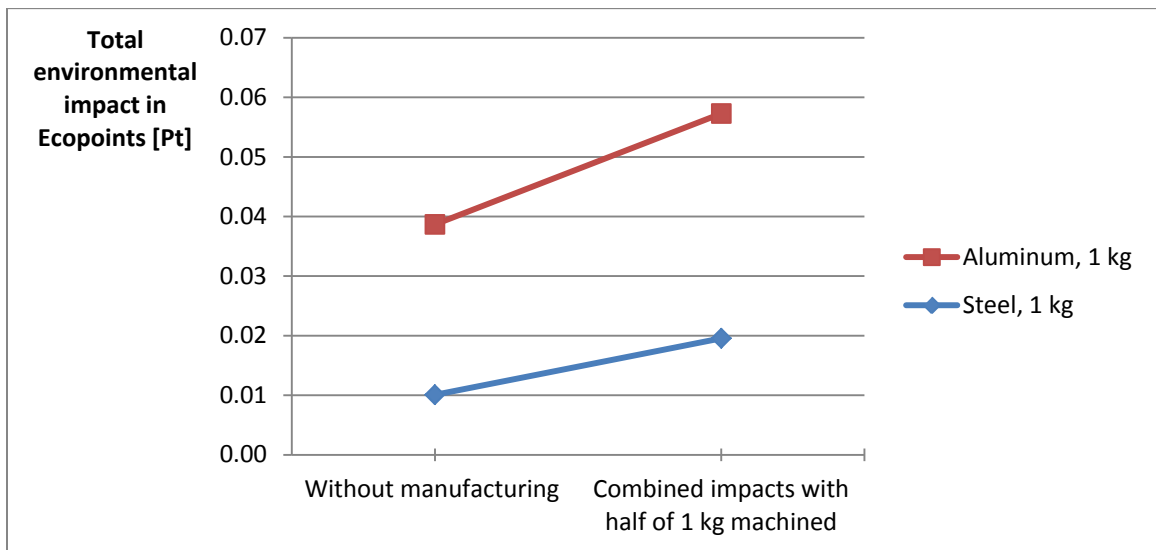


Figure 18: Example of impacts during a manufacturing stage

Sustainable Manufacturing is certainly also an important consideration during a design process [3,96] and an emerging topic of research [97,98]. However, for the purposes of selection of the optimal main components during the early design stages, it can be most efficient to exclude the manufacturing stage from the metamodels of environmental impact attributes at the conceptual design stage, and instead, include fewer and more viable options at later design iterations. By doing so, the environmental impact metamodels reduce to a design space of all

potential material alternatives. It becomes necessary to identify a unit basis on which all such data points can be modeled together.

7.1.3. Consistent modeling to represent units in a design space

An LCA process begins with the first step of identification of the goal and scope of a process [29]. 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 modeled 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 [99] 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.

7.1.3.1. Consideration of composite materials and sets of components

Products today are often made from composite materials, which are a composition of two or more materials that may have representative data available. 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 (10) 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

$$DS_{ij} = \left(\sum_{k=1}^p EIP_{jl} \Lambda_{ik} \right) VE_i \quad (10)$$

where j is one of fourteen different environmental parameters, k represents each of the materials in a composite, l is a material type that can be selected from among seventy-two different materials in a database, EIP_{jl} is the environmental impact parameter of a selected material l , Λ_{ik} is the volume 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 becomes 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, because 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 metamodels to identify optimal points where some potential unforeseen solutions could exist. The following subsection describes possible sources of the seed data that determine the values of the impacts in Equation (10).

7.1.3.2. Sources of environmental data

Data is available for the life cycle processes of a wide array of materials from sources such as ecoinvent [5]. Such databases are constantly expanding, but are not an exhaustive compilation of all data for every material. Ecoinvent is available to use as an independent source⁵ of information regarding material, energy, waste, and emissions flows that result from various processes in a product life cycle. Ecoinvent and other databases can also be included with simulation software such as SimaPro [30] or GaBi [93]. Results presented in this paper were

⁵ <http://www.ecoinvent.org/database/>

obtained by the use of ecoinvent data within SimaPro software. The purpose of this paper is to prescribe a methodology to use such data. It is recommended that a user obtain such access to the associated data for the most accurate and robust results. The following section outlines the steps to initiate the use of the methodology.

7.2. Rationale for Problem Formulation

Section 7.1.2 summarized both the credible LCA modeling approaches that have been developed by domain experts in recent years and the most significant associated considerations during the early stages of product design. An LCA model maps the flows of any substances that result from the processes that occur during any defined portion of a product life cycle. The prior section reduced the model considered by this approach to the selection of a single variable of the

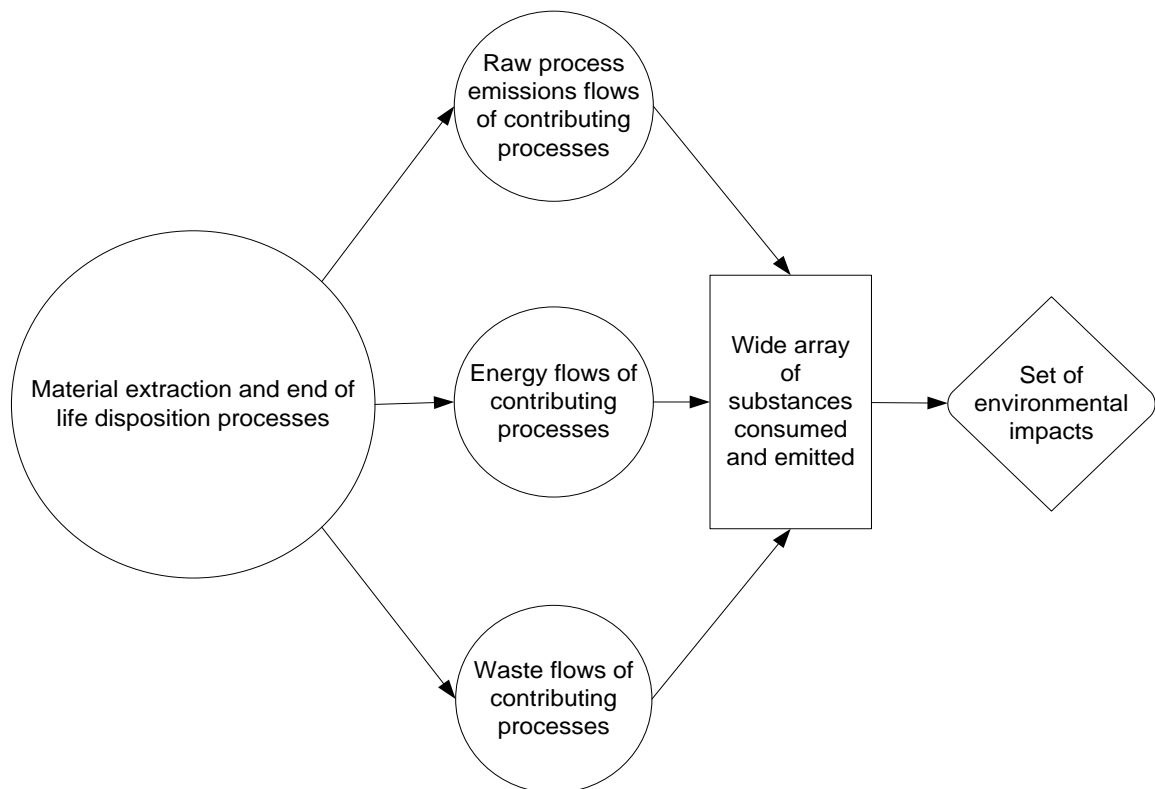


Figure 19: Mapping of the LCA process from the material selection perspective

material type of the main components and its associated mass or solid volume quantity. However, Figure 19 shows that each material option has a set of numerous contributing processes and many corresponding substances emitted. The mapping of the LCA process computes the resulting environmental impacts on the planet, humans, and other species. However, the specific groups of environmental impacts and the corresponding computational structures vary depending upon which Life Cycle Impact Assessment (LCIA) method is selected. The following subsection identifies several of the most widely used methods and some of the relative advantages of these various methods.

7.2.1. Selection of a Life Cycle Impact Assessment (LCIA) method to represent

Seminal works by Wenzel and Hauschild [26,100] introduced a methodology for the Environmental Design of Industrial Products (EDIP). This method uses a midpoint approach to compute the magnitudes of various categories of environmental impacts from the substances emitted and resources consumed throughout the product life cycle. Here, nineteen different categories of environmental impacts were identified. Of these nineteen, fifteen of the impacts are weighted for direct comparison to each other based on the relative severity to the planet, people, and species. There is no such capability for the remaining impact categories of nonrenewable resource consumption and three different forms of ecotoxicity. Other impact assessment methods include CML2001 [101], Eco-indicator 99 [101], IMPACT 2002+ [102], ReCiPe [103], and TRACI [104]. The approach of this paper focuses holistically on the mapping of factors to environmental impact responses and the aggregation of the multiple impacts with other attributes. The method described in this paper could represent any of these impact assessment methods. The 2003 version of EDIP was deployed to develop the method presented here.

7.2.2. Environmental impacts as design attributes

Multi-criteria decision making (MCDM) methods were prescribed to evaluate design alternatives for traditional design [7,8,10.43]. The Life Cycle Impact Assessment methods, which are described in the prior section, model environmental impacts into a form that can be represented as criteria in an MCDM model. Prior work introduced an approach to integrate LCA models into such a framework for engineering design [46]. This work builds on that prior work by introducing a method to represent an entire design space to select specific optimal sets of main components of a product. This approach provides the mathematical rigor of MCDM methods to the design of products for sustainability. The various environmental impact categories derived by the different Life Cycle Impact Assessment methods pose some key questions about how environmental criteria should be represented in an MCDM model.

7.2.2.1. Total environmental impact vs. most critical impact

Section 3.1 introduced the Environmental Design of Industrial Products (EDIP) of 2003. Since fifteen of the nineteen environmental impact categories represented by the EDIP method are weighted based on severity relative to each other, the weighted sum of these fifteen impacts may be considered as a single important criteria, or as an objective to minimize. These impacts are all expressed in the common units of Ecopoints [Pt], as Section 2.2 points out. The magnitude of Ecopoints can often vary widely across this set of fifteen different impacts. Thus, those with the highest magnitude could be considered those with the greatest priority for reduction. Such a preference could also depend upon other considerations such as the typical profile of impacts for that product family, or any differences in the severity profile of the geographic region where that product is likely to be localized. The impact that has the greatest magnitude is likely to vary for each design alternative. Thus, a single attribute of the most severe impact would likely be difficult to represent by a single model due to the different mapping of the different impacts to their factors. Utility theory provides a mathematically rigorous structure to formulate such

preferences among multiple attributes and the risk preferences for each single attribute. Utility theory has been successfully prescribed for and applied to traditional engineering design problems with multiple objectives in recent years [45,105]. Thus, each environmental impact can be modeled as an attribute in such a formulation.

The remaining impacts of nonrenewable resource consumption and the three different forms of ecotoxicity would need to be aggregated as separate attributes. The EDIP method has no prescription to weigh these impacts based on severity relative either to each other or to the other fifteen impacts. However, these impacts can be represented as different attributes in a multi-attribute utility formulation. Ecotoxicity may exist in the forms of either that which is acute in water, chronic in water, or chronic in soil. It may be difficult for a design engineer to express preferences among these three different forms of ecotoxicity. However, prior published historical data may help to inform the decision maker and perhaps suggest preferences for consideration and modification if necessary.

Such historical data appears in the work of Kietzmann [100]. The data identifies 1990 actual levels and desired political target levels in a region of study. From these values, the percent of reduction desired can be calculated. Here again, preferences can change in different locations and at different times. If one may assume for the purposes of product design that this percent of reduction desired is consistent with the relative preferences to minimize these three impacts, the percentages can be converted into a normalized set of weights for the multi-attribute utility formulation of ecotoxicity as shown in Table 10. These weight values should be adjusted as the values of actual and desired levels change over time. Here again, the purpose is to provide some baseline to model the preferences for engineering design and not to prescribe any new Life Cycle Impact Assessment method. Once such preferences are modeled, the model of the main environmental attribute would consist of the preference model among ecotoxicity, nonrenewable resources consumption, and the aggregation of the fifteen impacts that are weighted relative to each other based on severity. Since design for sustainability requires more than just the

environmental considerations, a model would need to be extended to include other categories of product attributes.

Table 10: Estimation of preference weights for an ecotoxicity attribute

Ecotoxicity category	Actual level in 1990 [100] [cu.meter/person/year]	Political target level desired [100] [cu.meter/person/year]	% reduction of actual desired	Preference weights based on relative percent reduction desired
Water, acute	38000	15000	60.5%	0.329
Water, chronic	420000	170000	59.5%	0.323
Soil, chronic	120000	43000	64.2%	0.348

7.2.3. Life Cycle Cost and product performance attributes

A sustainable design should consider any effects on the people, planet, and profit [2,4]. Examination of these effects across an entire design space should include a data 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 19 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 maximize the benefits to the people, planet, and profit.

Figure 20 shows the mathematical construction of such a multi-attribute utility formulation. Here, the construction of metamodels can expand the exploration of the entire design space. This process is covered more in depth in the following two sections. Initially, the design space can be represented by sets of data points associated with design alternatives, where each point includes all attributes and associated factors, or independent variables.

7.2.3.1. The question of independence of the multiple attributes

The attributes in a multi-attribute utility formulation should be independent from each other to facilitate the problem formulation [8,106,107]. A multi objective problem exists where, in some examples, such as a beam deflection problem, a tradeoff may exist between attributes [7,107] such as cost and strength. Such a situation can result in a Pareto optimal frontier, where

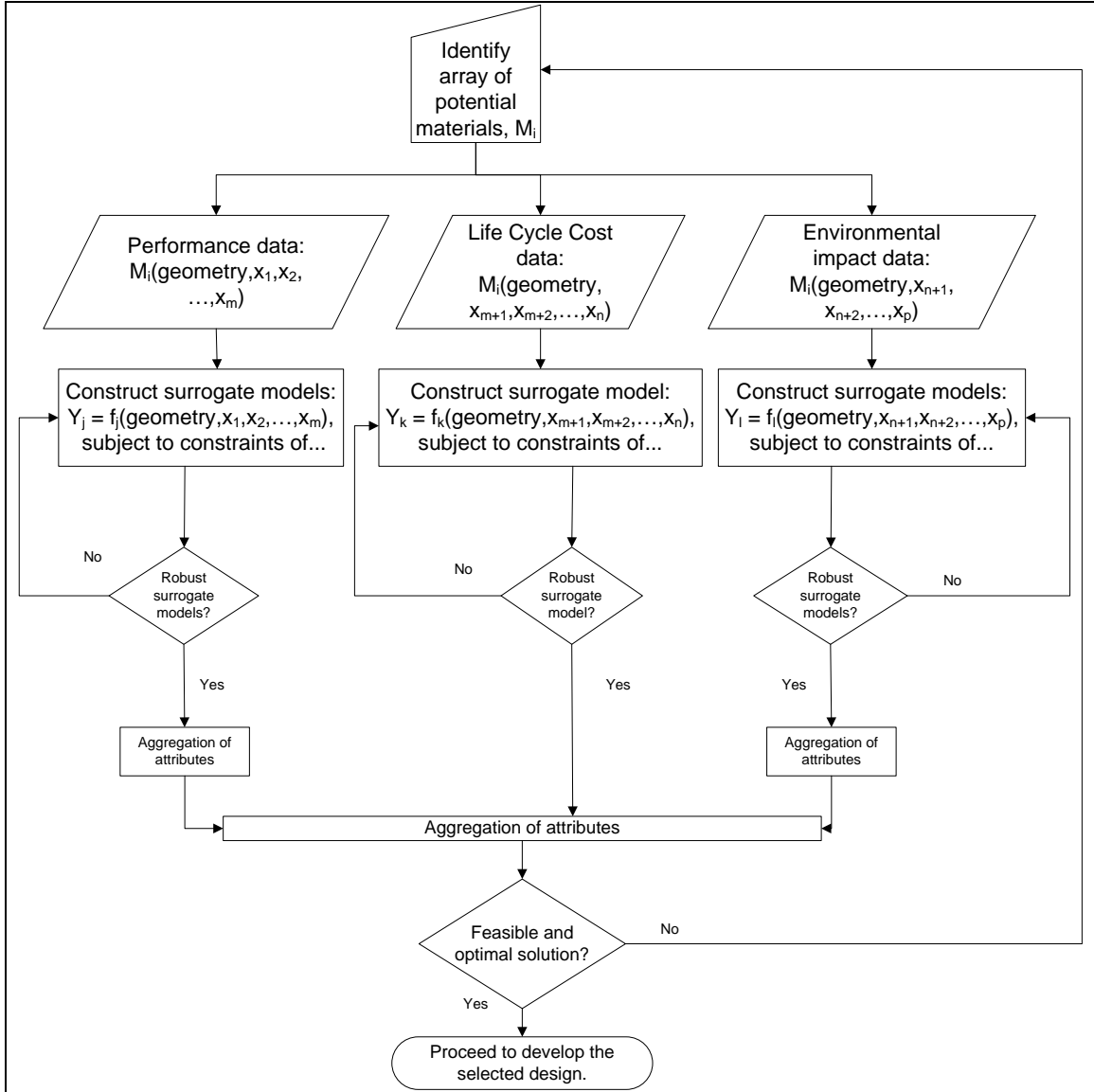


Figure 20: Methodology for a Robust Surrogate Modeling Approach for Material Selection in Sustainable Design of Products (MASSDOP)

the optimal solution is at the intersection of that Pareto optimal curve and a vector that represents the weighted preferences among the attributes. Linear correlations and regression models or other metamodels can help to identify such relationships between attributes and also to identify which independent variables affect which of the 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 is a measure that could be used to find the shortest distance in the vector space of a given alternative to the optimal. This computation would also reveal which of the independent variables would need to change to find a new material that could be closer to the optimal solution than could be realized by looking at only the original design set.

7.2.3.1.1. Mechanical properties relationship to environmental impacts

The problem of material selection raises some questions to consider regarding the multiple attributes that represent sustainability. Performance attributes in traditional design for material selection usually depend upon various mechanical properties of the materials in a set of alternatives. A key question concerns whether these same mechanical properties can be used to map to attributes such as environmental impact. Table 11 compares the results of mapping mechanical properties to those of mapping the environmental properties of contributing processes during a life cycle with the goal of estimating the total environmental impact. This study considers a limited data set for one kilogram quantities of six different metals. The results show that there is potential to model impacts as a function of normalized values of the mechanical properties of materials. However, such models are likely to be less accurate than those which express impacts as a function of the contributing processes in the life cycle of the one kilogram of material. The importance of accuracy and the techniques for metamodel construction and the specific meanings of the independent variables that represent contributing processes will be covered in the following two sections. In a utility-based model, it becomes possible to model each

attribute as a function of the independent variables upon which an attribute is affected the most.

Therefore, the following section describes a method to create more accurate relationships to model environmental impacts.

Table 11: Investigation of mapping environmental impact from mechanical property variables

	1 kg	Low alloy steel	300 series stainless steel	Cast iron	Aluminum	Tin	Copper	
Total sum (Output response) = sum of all input variables	Pt units	0.0101	0.0220	0.0122	0.0387	0.1007	0.1750	
Remaining processes percentage of total impact		16.57%	21.79%	10.91%	21.73%	14.91%	1.45%	
Prior cut off value			1.50%		1.20%			
Maximum remaining processes value for 12% of total impact		0.0012	0.0026		0.0046	0.0121		
New cut off value			0.57%		0.41%			
Resulting surrogate model of environmental independent variables:								
Y = 0.01214444 + -0.00185018*A + -1.890768*C*C + 2428.74*H*H + 442.1518*A*C + -1138.47*A*F								
Y Output values predicted by surrogate model		0.0101	0.0220	0.0122	0.0387	0.1007	0.1750	
Error = Actual Y - Predicted Y		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
% Error		0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	
Mechanical properties								
Yield strength	MatWeb	MPa	711	458	428	69.6	14	222
Modulus of Elasticity	MatWeb	GPa	204	195	147	68.4	44.3	116
Poisson's ratio	MatWeb		0.29	0.281	0.287	0.33	0.33	0.31
Weight density	MatWeb	kg/m ³	7850	7830	7240	2700	7290	8930
Ultimate tensile strength	MatWeb	MPa	989	742	503	111	220	318
Shear modulus	MatWeb	GPa	79.8	77.9	58.1	25.9	15.6	44
Charpy impact	MatWeb	J	56.3	157	15.3			
Brinell Hardness	MatWeb		276	187	299	32.1	3.9	
Machinability	MatWeb	%	59.8		39	20		20
Fatigue Strength	MatWeb	MPa	472	369	260	42.6		89.6
Specific heat	MatWeb	J/g-°C	0.475	0.497	0.506	0.901	0.256	0.385
Thermal conductivity	MatWeb	W/m-K	46.4	15.4	26.6	229	62	390
Resulting surrogate model of mechanical properties:								
Y = 0.08601715 + -0.0009053282*Modulus of Elasticity*Specific heat + 3.667327E-08*Weight density*Thermal conductivity								
Y Output values predicted by surrogate model		0.0116	0.0027	0.0257	0.0529	0.0923	0.1733	
Error = Actual Y - Predicted Y		-0.0016	0.0193	-0.0136	-0.0142	0.0084	0.0017	
% Error		16%	88%	112%	37%	8%	1%	
Mechanical properties normalized linearly								
Yield strength	MatWeb		1.00	0.64	0.59	0.08	0.00	0.30
Modulus of Elasticity	MatWeb		1.00	0.94	0.64	0.15	0.00	0.45
Poisson's ratio	MatWeb		0.18	0.00	0.12	1.00	1.00	0.59
Weight density	MatWeb		0.83	0.82	0.73	0.00	0.74	1.00
Ultimate tensile strength	MatWeb		1.00	0.72	0.45	0.00	0.12	0.24
Shear modulus	MatWeb		1.00	0.97	0.66	0.16	0.00	0.44
Specific heat	MatWeb		0.34	0.37	0.39	1.00	0.00	0.20
Thermal conductivity	MatWeb		0.08	0.00	0.03	0.57	0.12	1.00
Resulting surrogate model of normalized mechanical properties:								
Y = 0.09459703 + 1.23379E-05*Specific heat + 0.1828472*Yield strength*Weight density + -0.699115*Yield strength*Specific heat + -0.003823195*Weight density*Shear modulus + 0.06916236*Weight density*Thermal conductivity								
Y Output values predicted by surrogate model		0.0099	0.0211	0.0125	0.0388	0.1009	0.1749	
Error = Actual Y - Predicted Y		0.0001	0.0009	-0.0003	-0.0002	-0.0002	0.0001	
% Error		1.35%	4.15%	2.44%	0.41%	0.20%	0.04%	

7.3. Mapping Input Factors to Attribute Outputs

This section covers the process by which data sets can be formed to use for the surrogate model construction that is presented in the following section. The prior section summarized such a potential method to model performance attributes as a function of mechanical properties of materials as described in previous works pertaining to traditional engineering design [108]. Sections 7.1.3.1 and 7.2.3 summarized a similar process to construct life cycle cost models. Figure 19 illustrates the mapping of life cycle processes of a given material to their environmental impacts. This process is complicated more so in the case of environmental impacts than in the case of cost and performance attributes by the large number of factors upon which the environmental impacts depend. The following subsection addresses this issue by introducing a novel approach to mitigate this complication.

7.3.1. The issue of dimensionality in Life Cycle Assessment (LCA)

The Life Cycle Assessment (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, a significant number of both the numerous processes and substances contribute relatively insignificant quantities to environmental impacts. Furthermore, all of the significant contributing processes were found to fit into a much smaller number of broader categories of processes. These two key topics are addressed specifically in the following two subsections.

7.3.1.1. Factor significance tradeoff between dimensionality and model accuracy

Any model that depends upon several hundred different variables would be difficult to work with. The question then concerns how many of the variables with low quantity can be added into a residual variable category called “Remaining processes”. One approach could be 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 the total for the sum of the remaining processes. The top portion of Table 11 shows that a limit of twelve per cent for the sum of the remaining processes, for six different materials in that data set, kept the remaining processes variable to a low level of significance in a metamodel constructed by second order polynomial regression. It is important to limit the significance of the remaining processes variable in any model, because it is a residual term. Significance of any residual term, such as error, could affect the accuracy and predictability of the model. However, if this residual term is reduced by too much, the number of variables could be too numerous to include for model construction and optimization. The construction of a meaningful model could also be compromised when there are fewer than three variables. The specific heuristic that was used to establish the cutoff amount for each data point is shown in Figure 21. A maximum safe limiting target value of 11% of an attribute was estimated for the residual variable of the total remaining processes after the cut off operation. This estimate was

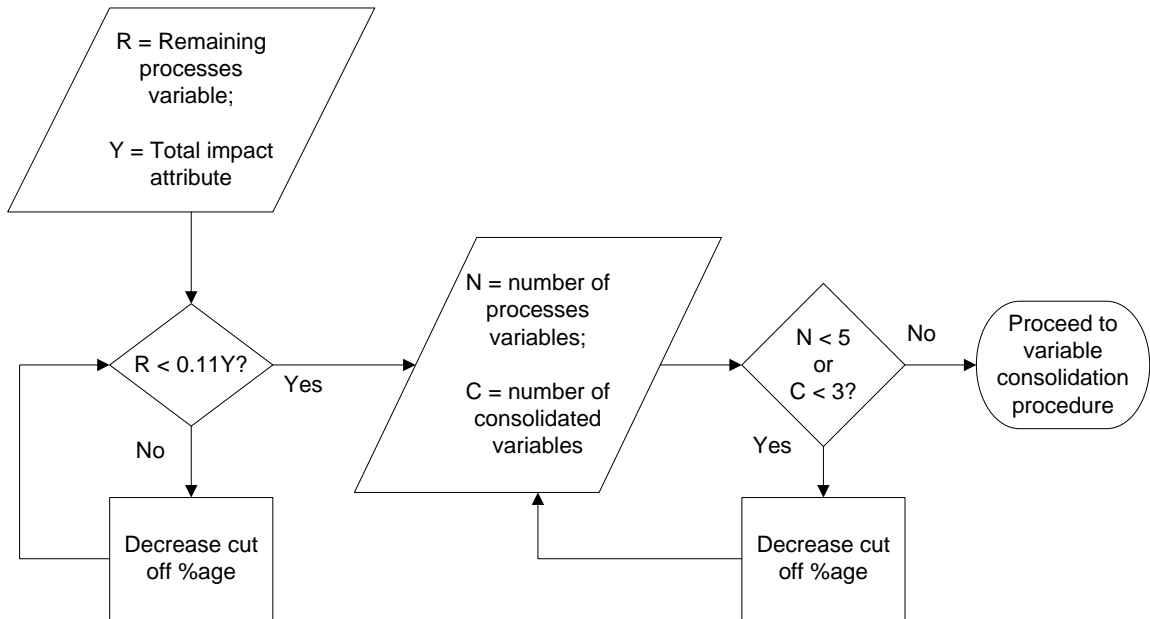


Figure 21: Process to include significant variables

obtained by the results of a limited empirical test to achieve one accurate model, as shown in the top of Table 11. The following subsection describes a process to address this issue of dimensionality.

7.3.1.2. Consolidation of many factors

The process described in the prior subsection reduces the number of variables from several hundred down to anywhere from several to about thirty depending upon the category of environmental impact and the material that the LCA computation is generated for. The larger number of variables could still be too difficult to use and the variables that appear as significant can change from one material to another. However, 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 12. 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 19. Thus, further reduction in the number of variables is achievable, but that would limit the amount of specific information compared to the dozen variables shown in Table 12.

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 four 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. Fourth, sums are entered as the associated variable value. Figure 22 shows the succession of these process steps. Table 13 shows an actual example of how one of these data points was generated using this process. Contributing processes and substances can both be expressed in weighted units

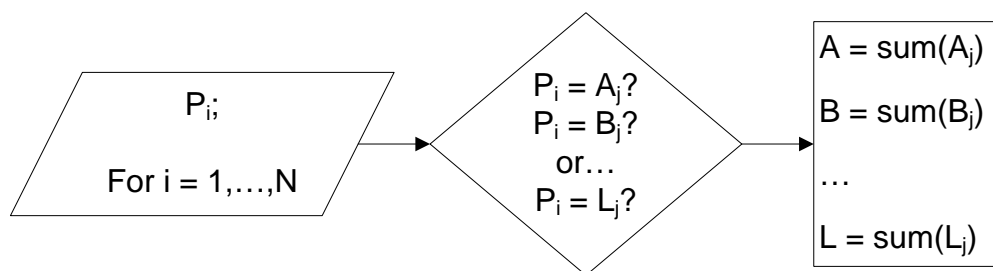


Figure 22: Process to consolidate environmental parameters

Table 12: Descriptions of consolidated environmental variable categories

Total sum (Output response) = sum of all input variables	Y	[5,30]	Pt
Process		Project	Unit
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, sulfidic 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

of Ecopoints [Pt]for consistent comparisons. The value of the residual variable of remaining processes is labeled as R and was computed by the procedure described in the prior subsection. A final check should be done to add the Pt values of variables A through L together along with the

Table 13: Example of the variable consolidation process implemented by sort and sum

No	Process	Project	Unit	Total	Variable category
19	Silicon carbide, at plant/RER WITH US ELECTRICITY U	US-EI 2.2	Pt	0.00099	A
5	Uranium, enriched 3.8%, at USEC enrichment plant/US WITH US ELECTRICITY U	US-EI 2.2	Pt	0.00027	B
16	Radioactive waste, in final repository for nuclear waste SF, HLW, and ILW/CH WITH US ELECTRICITY U	US-EI 2.2	Pt	0.00059	B
21	Radioactive waste, in final repository for nuclear waste LLW/CH WITH US ELECTRICITY U	US-EI 2.2	Pt	0.00131	B
8	Disposal, sulfidic tailings, off-site/GLO WITH US ELECTRICITY U	US-EI 2.2	Pt	0.00029	C
25	Disposal, spoil from coal mining, in surface landfill/GLO WITH US ELECTRICITY U	US-EI 2.2	Pt	0.01046	D
11	Process-specific burdens, sanitary landfill/CH WITH US ELECTRICITY U	US-EI 2.2	Pt	0.00036	E
13	Process-specific burdens, residual material landfill/CH WITH US ELECTRICITY U	US-EI 2.2	Pt	0.00046	E
14	Disposal, hard coal ash, 0% water, to residual material landfill/DE WITH US ELECTRICITY U	US-EI 2.2	Pt	0.00049	F
23	Disposal, spoil from lignite mining, in surface landfill/GLO WITH US ELECTRICITY U	US-EI 2.2	Pt	0.00271	G
4	Hard coal, burned in power plant/SPP WITH US ELECTRICITY U	US-EI 2.2	Pt	0.00024	H
7	Hard coal, burned in power plant/MRO WITH US ELECTRICITY U	US-EI 2.2	Pt	0.00029	H
9	Hard coal, burned in power plant/WECC WITH US ELECTRICITY U	US-EI 2.2	Pt	0.00035	H
20	Hard coal, burned in power plant/SERC WITH US ELECTRICITY U	US-EI 2.2	Pt	0.00124	H
22	Hard coal, burned in power plant/RFC WITH US ELECTRICITY U	US-EI 2.2	Pt	0.00154	H
6	Blasting/RER WITH US ELECTRICITY U	US-EI 2.2	Pt	0.00028	I
1	Natural gas, at consumer/RNA WITH US ELECTRICITY U	US-EI 2.2	Pt	0.00021	J
2	Natural gas, sour, burned in production flare/MJ/GLO WITH US ELECTRICITY U	US-EI 2.2	Pt	0.00023	J
3	Operation, freight train, diesel/RER WITH US ELECTRICITY U	US-EI 2.2	Pt	0.00024	J
10	Crude oil, at production onshore/RAF WITH US ELECTRICITY U	US-EI 2.2	Pt	0.00036	J
15	Natural gas, at production/RNA WITH US ELECTRICITY U	US-EI 2.2	Pt	0.00053	J
17	Crude oil, at production onshore/RU WITH US ELECTRICITY U	US-EI 2.2	Pt	0.00059	J
18	Crude oil, at production onshore/RME WITH US ELECTRICITY U	US-EI 2.2	Pt	0.00085	J
12	Disposal, inert material, 0% water, to sanitary landfill/CH WITH US ELECTRICITY U	US-EI 2.2	Pt	0.00037	L
24	Disposal, hard coal ash from stove, 0% water, to sanitary landfill/CH WITH US ELECTRICITY U	US-EI 2.2	Pt	0.00403	L
	Remaining processes		Pt	0.00344	R
	Total of all processes		Pt	0.03270	Y
				Sum of variable	
				0.00217	B
				0.00082	E
				0.00367	H
				0.00300	J
				0.00440	L

value of R. The total sum should be equal to that environmental impact's total value in Pt if the procedure was executed correctly. The scalability of the mapping of all these variables was confirmed by a test of one material.

7.3.2. Aggregation of attributes for Multi-Criteria Decision Making (MCDM)

Section 7.2.2.1 described the nineteen different environmental impact categories and groupings for weighted comparisons as defined by the Environmental Design of Industrial Products (EDIP) [26]. Here, a decision maker should articulate the preferences among these nineteen attributes, and the preferences should be modeled consistently. Various utility-based methods have been prescribed to achieve consistent preference modeling [10,45,109]. The large number of nineteen attributes poses a challenge that remains a topic for further research. However, the fact that the EDIP method does provide weighting based on severity for fifteen of these nineteen impacts could help. The total impact of these fifteen is computed during the LCA process by using this weighting into an aggregated attribute named the Single Score [94]. Thus, the remainder of this paper will focus on the modeling of this single score attribute, because the procedure to create the model for any other environmental impact would be the same as is described in this section.

However, an open question posed in Section 7.2.2.1 concerns a scenario in which a decision maker may prioritize minimization of the worst or highest magnitude environmental impact among the fifteen different impacts. Table 14 provides an initial view of model accuracy and predictability that may be expected when models are created for specific highest magnitude impacts. The table shows results from models constructed by both second order polynomial regression and Kriging method. This test indicated that the accuracies of the models are significantly better when specific impacts are modeled on their own instead of mixed with others. This suggests a limitation to consider when the goal is to minimize the highest magnitude

impacts. Alternatively, each impact could be modeled as a single attribute. Section 7.2.2.1 suggests a method to aggregate the remaining four of nineteen impacts into a decision model.

7.3.3. Representation of parametric uncertainty

Uncertainty of environmental data is another important issue to take into account [38]. Ecoinvent provides a formulation to do so [5]. Software such as SimaPro is capable of estimating the uncertainty bands of all the impacts by executing Monte Carlo simulations based on the

Table 14: Initial model tests of highest magnitude environmental impacts

Surrogate Model Construction of Greatest Environmental Impacts for 1 kg Unit of Each Material Summary of Results													
Greatest impact Group	Number of materials in the group	Number of materials used for model construction	R-sq adjusted %age precision of model from PR	Significance of residual variable, R, in PR model equation	Number of variables in model	R-sq adjusted %age precision of model from Kriging	First test material for model validation	Error between first test material and PR model % of actual	Error between first test material and Kriging model % of actual	Second test material for model validation	Error between second test material and PR model %	Error between second test material and Kriging	Potential uses
Aquatic eutrophication EP(P)	29	11	100%	Moderate	5	31.9%	Brass	0.0%	-0.2%	Magnetite	0.0%	0.6%	Both models look very promising.
Human toxicity water	21	7	100%	Moderate to High	4	88.4%	Nylon 6	0.6%	-28.0%	HDPE granulate	109.8%	133.5%	This may need some additional segregation to model by material group too.
Human toxicity water	This is the 3rd and 4th validation test for this attribute.						Zinc	-35.8%	1.2%	PVC	-4.1%	-15.0%	Aside from the outlier material, the PR model may be usable but with a fairly high variance.
Human toxicity water	21	11	100%	Moderate	5	67.50%	Polyester resin glass fiber reinforced hand lay up	-37.4%	0.9%	Polystyrene GPPS	-18.6%	-0.2%	This test adds 4 data points into the model.
Acidification	6	2	100%	Low to moderate	6	24.80%	Green veneer plywood	0.0%	1.3%	Oriented strand board	30.0%	-1.8%	Greater model uncertainty for this group is likely due to small groups of more disparate data.
Ozone formation (Human)	3	1											
Slags and ashes	1	1											
Bulk waste	7	2											
Ozone depletion	2	2											
Human toxicity air	5	2											

distributions of substances emitted during life cycle processes. Prior work [46] demonstrates that accounting for uncertainty in both environmental and cost attributes can influence which alternative is selected. Although mean values are presented in this paper, expected utility formulations can provide effective methods to simultaneously consider both utility and probabilistic uncertainties [44,110]. The best use of such methods for sustainability remains a topic for further research. In addition to uncertainty in data, uncertainty in a surrogate model, or approximate model, is another important consideration. The following section covers topics related to the construction of the surrogate models.

7.4. Surrogate Model Construction

The first step in the construction of a surrogate model is to generate a set of data points consisting of the values of all independent variables and their associated attributes or responses. Such a data set was generated for the single score, or total environmental impact, of a diverse array of seventy-two different materials by using the method introduced in the prior section. This data set was extracted from the Life Cycle Assessment in units of Ecopoints [Pt] [30] per kilogram of each of the materials. All values were converted to units of Pt per cubic meter by multiplying by the mass density of each material as recommended in Section 7.1.3. 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. The following subsection introduces a novel approach to identify a sample set.

7.4.1. Design space filling

Data that represents material properties poses a unique challenge for the construction of a surrogate model. Data related to materials has 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 [111,112] require strategic data locations that are uniform and balanced. The challenge is to find a way to approximate a viable space filling method to optimize model accuracy and robustness given the inherent limitations. Material selection could introduce some potential for groupings based on common characteristics within groups of materials. The following subsection highlights such an investigation.

7.4.1.1. Potential for stratified sampling

Ashby introduced charts [108] to identify groups of materials based on locations in a design space as defined by mechanical property values for traditional design. Figure 23 shows a similar grouping identified based on environmental properties. Here, four groups were segregated based on the single score, which is the third axis not shown here. A three dimensional chart would show four different bubbles in separate locations in that space. The interesting differences between the groups are the ranges of the percentage of the top two environmental impacts of the total impacts and the percentage that impacts from the end of life stage of the life cycle are of the

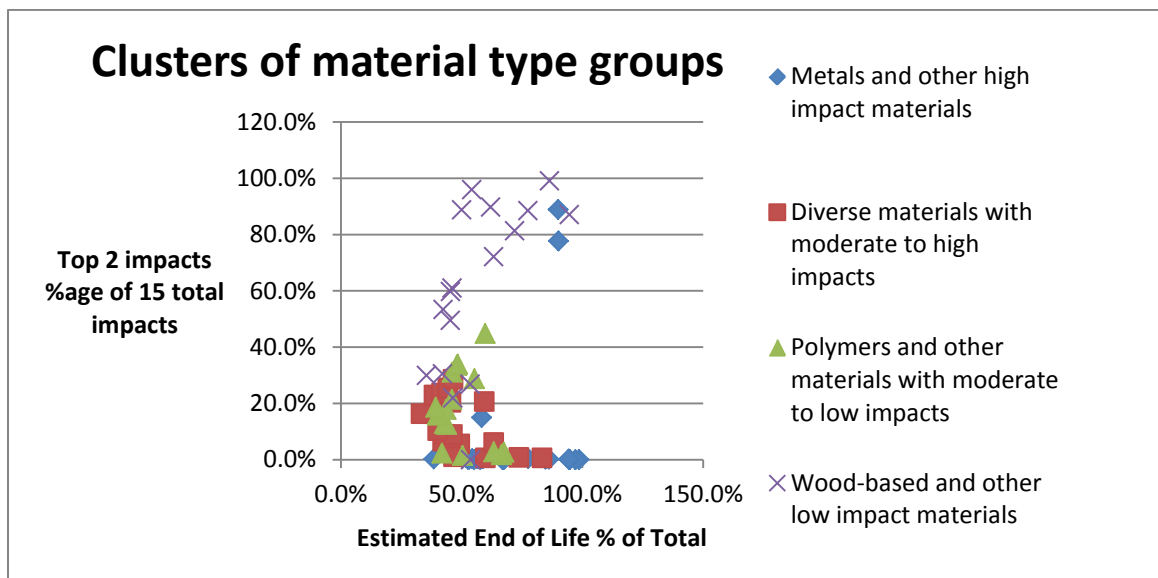


Figure 23: Materials stratified into groups with separate ranges of total environmental impact

Table 15: List of materials to choose from in a data set

Material extraction process for 1 kg of:	Material extraction process for 1 kg of:
Aluminium alloy, AlMg3, at plant	Limestone, milled, packed, at plant
Aluminium, primary, at plant	Lithium, at plant
Antimony, at refinery	Magnesium, at plant
Asbestos, crysotile type, at plant	Magnesium-alloy, AZ91, at plant
Bauxite, at mine	Magnetite, at plant
Brass, at plant	MG-silicon, at plant
Brick, at plant	Mischmetal, primary, at plant
Bronze, at plant	Molybdenite, at plant
Cadmium, primary, at plant	Nickel, 99.5%, at plant
Carbon black, at plant	Nylon 6, at plant
Cast iron, at plant	Nylon 6, glass-filled, at plant
Sanitary ceramics, at regional storage	Nylon 66, at plant
Charcoal, at plant	Nylon 66, glass-filled, at plant
Chromium steel 18/8, at plant	Oriented strand board product
Clay, at mine	Palladium, primary, at refinery
Cobalt, at plant	Pig iron, at plant
Cold rolled sheet, steel, at plant	Platinum, primary, at refinery
Concrete block, at plant	Plywood, at plywood plant
Copper, primary, at refinery	Polybutadiene, at plant
Corrugated board, mixed fibre, single wall, at plant	Polycarbonate, at plant
Dry veneer, at plywood plant	Glass fibre reinforced plastic, polyester resin, hand lay-up, at plant
Epoxy resin, liquid, at plant	Polypropylene resin, at plant
Polystyrene, expandable, at plant	Polystyrene, general purpose, GPPS, at plant
Ferrite, at plant	Polystyrene, high impact, HIPS, at plant
Ferrochromium, high-carbon, 68% Cr, at plant	Polyurethane, rigid foam, at plant
Ferromanganese, high-coal, 74.5% Mn, at regional storage	Polyvinylchloride, at regional storage
Ferronickel, 25% Ni, at plant	Rhodium, primary, at refinery
Flat glass, uncoated, at plant	Iron scrap, at plant
Glass fibre, at plant	Silicon carbide, at plant
Gold, primary, at refinery	Silicone product, at plant
Graphite, at plant	Silver, from combined gold-silver production, at refinery
Green veneer, at plywood plant	Steel, low-alloyed, at plant
High density polyethylene resin, at plant	Synthetic rubber, at plant
High impact polystyrene resin, at plant	Tetrafluoroethylene, at plant
Iron-nickel-chromium alloy, at plant	Tin, at regional storage
Dry rough lumber, at kiln	Titanium zinc plate, without pre-weathering, at plant
Laminated veneer lumber, at plant	Uranium natural, at mine
Linear low density polyethylene resin, at plant	Zinc, primary, at regional storage
Lead, primary, at plant	Zinc oxide, at plant

total impacts, shown as the two axes in Figure 23. This information could be useful to a decision maker when articulating the preferences among environmental impacts as explained in Section 7.3.2. However, Table 16 compares, based on some random sampling, modeling of each group in isolation to modeling of four of the five groups consolidated into one main group. The groups are labeled A through D with A having the highest environmental impact and D the lowest. The

Table 16: Comparison of model construction with and without stratification

Surrogate Model Construction for Total Environmental Single Score for 1 kg Unit of Material Summary of Results													
Material Group	Number of materials in the group	Number of materials used for model construction	R-sq adjusted %age precision of model from PR	Significance of residual variable, R, in PR model equation	Number of variables in model	R-sq adjusted %age precision of model from Kriging	First test material for model validation	Error between first test material and PR model % of actual	Error between first test material and Kriging model %	Second test material for model validation	Error between second test material and PR model %	Error between second test material and Kriging	Potential uses
Very High Impact	6	5	100%	Moderately High	4	54.8%	Palladium	1.1%	107.0%	NA	NA	NA	PR model should be adequate to roughly estimate this suboptimal region.
A	23	10	100%	Moderate	10	53.4%	Zinc	5.8%	249.4%	Brass	1.4%	58.8%	PR model only
B	17	6	100%	Moderate	6	81.1%	Nylon 6	-23.5%	8.8%	Oriented strand board	62.5%	-2.2%	Kriging model only
C	16	5	100%	Moderate	5	9.7%	Polyvinylchloride PVC	-14.4%	2.1%				Kriging better so far, but the Rsq is a concern.
D	17	7	98.4%	Very high	1	99.6%	HDPE granulate	NA	-60.5%	Green veneer plywood	NA	-47.4%	Not recommended
Groups B and C	33	11	98.8%	Very low	6	88.1%	Nylon 6	-55.7%	-17.0%	Polyvinylchloride PVC	4.5%	5.7%	Not as good as separated group models
Groups A, B, and C	56	21	100%	Fairly low	11	41.3%	Zinc	-0.7%	-1.4%	Nylon 6	-93.0%	34.6%	Maybe better for Group A than for Group C
Groups A through D	73	28	100%	Very low	13	22.8%	HDPE granulate	8.0%	-23.3%	Zinc	-0.5%	-5.1%	PR model looks best so far, and this single model may be the best overall.
Groups A through D combined on a volume unit basis	73	28	100%	Low	11	37.1%	HDPE granulate	35.0%	3.0%	Zinc	-3.9%	-3.1%	This scaling adjustment may have some effect on model accuracy.

results show that potential model accuracy should be better when the groups are modeled together. The population size of the data is significantly reduced when the stratified groups are modeled separately. One small group that was not included contained just six materials that all had unusually high impacts. That group was not included both for reasons of scalability and for the very low likelihood that such materials could ever be optimal for a sustainable design. Table 15 shows the specific life cycle process of material extraction used to generate data for all of the seventy-eight different materials that could be selected to model a design space. The next subsection discusses potential options to select an initial sample set.

7.4.1.2. Space Filling Sampling (SFS)

Random sampling could have unpredictable results. One study compared the use of random sampling, stratified sampling, and Latin Hypercube [113]. All three approaches have some degree of randomness. A Latin Hypercube design requires space filling with data in specific cell locations, but the location within each cell is randomized. This study by McKay and associates [113] found Latin Hypercube to usually be at least as accurate for the examples studied in comparison to both random sampling and stratified sampling. Thus, Latin Hypercube becomes the most obvious choice for this situation of nonflexible data locations for material alternatives. Even with multiple generations of Latin Hypercube 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 minimizes 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 seven-two materials are shown in Table 17. These results reveal that most all 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 limited to usually 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 randomization. Husslage and associates [114] pointed out three possible ways to increase the cell sizes of a Latin Hypercube design of: increase in the population size, decrease in the number of variables, and decrease in the number of sample points. The decrease in the number of sample points would be the opposite of what is needed here. Population size is limited by the amount of data or design alternatives in the set. A decrease in the number of variables is possible, but information about specific assignable causes would be lost in doing so. Thus, there is a limit to the size of the initial sample set. However, this limitation could be acceptable,

Table 17: Best sample 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

because prior studies [84,115-117] indicated that the best surrogate models could be constructed by a two stage process in some cases. The next subsection introduces a second stage for this process.

7.4.1.3. 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 [82,85,118] and are thus not applicable to this situation of material selection. The study conducted by Jin and associates [115] 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 modeling 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 and associates [115] compared these methods in six different examples. One of the examples is comparable to an environmental impact example in that it is nonlinear with a dozen variables. Maximin Distance outperformed cross-validation in four of the six examples, and Maximin Distance outperformed Maximin Scaled Distance in the nonlinear 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 prioritizes 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. The first study in this work examines the total single score environmental impacts in Ecopoints per cubic meter for all seventy-two different materials in the generated data set. The Latin Hypercube process presented in the prior subsection identified fourteen data points to use for the original sample set. The chart in Table 18 shows the ordered list of the Maximin distances computed for the remaining data points. Although twenty-two more points would be needed to fill the sample set with half of the data, only the first nine points in this example have significantly greater distances than other points. When the size of the remaining sample set increased from the nine data points to the top twenty-two 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

Table 18: Maximin distances for SIS prioritization

Index numbers of materials in the remaining design space	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

smaller number of sample points could have better prediction accuracy of the points that are not included in the model. Results will vary for different models of different data sets. Criteria for testing the models are covered more in depth in Section 7.4.3. The following subsection discusses potential methods to construct the surrogate models from the sample data sets created.

7.4.2. Response surface modeling methods comparison

Metamodel 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 [83-85,119,120]. Here again, the material selection situation is a different case. Kriging method uses information from the model to predict intermediate data location estimates. Kriging method improved model accuracy in some cases over second order polynomial regression where the number of variables was high [121,122]. Few studies have been done using Kriging in situations without uniform data locations.

Second order polynomial regression should improve the model for optimization purposes compared to the first order linear model that was described in Section 7.3.1.2. The second order model, unlike the flat plane of a first order model, would emphasize 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 (SOB) regions of a curve [89,123]. Therefore, this work compares the results of using both Kriging and second order polynomial regression methods for response surface modeling. For the example described at the end of the last subsection with a sample size of thirty-six points, the R-squared adjusted was 100% for the second order polynomial regression model compared to an R-squared adjusted of 28.64% for the Kriging model. For the same example with the sample size of twenty-three data points, the R-squared 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. So,

each model should be tested and evaluated individually. The following subsection covers testing criteria.

7.4.3. Model testing

A designer would need to evaluate whether or not a constructed approximate model is adequate to use to optimize for a given design situation. Research topics concern the accuracy of

Table 19: Original sample set after Latin Hypercube space filling sampling

From 2nd order Polynomial Regression											
DATA	Y	YHAT	RESIDUAL	StdR	StuR	Residual	% error	Absolute value of % error	Material	Y	Data point
1	0.1426823E+00003	0.1428457E+00003	-.1634086E+00000	-0.8381	-1.	-1.63E-01	-0.1%	0.1%	AlMg3	142.682	1
2	0.9665366E+00004	0.9665327E+00004	0.3904724E-00001	0.2003	0.	3.90E-02	0.0%	0.0%	Antimony	9665.37	2
3	0.3766261E+00003	0.3766122E+00003	0.1391075E-00001	0.0713	0.	1.39E-02	0.0%	0.0%	Cobalt	376.626	6
4	0.1021553E+00004	0.1021585E+00004	-.3217021E-00001	-0.1650	-0.	-3.22E-02	0.0%	0.0%	Iron nickel-	1021.55	16
5	0.3149437E+00003	0.3149419E+00003	0.1824527E-00002	0.0094	0.	1.82E-03	0.0%	0.0%	Lead	314.944	18
6	0.3809048E+00004	0.3809060E+00004	-.1201281E-00001	-0.0616	-0.	-1.20E-02	0.0%	0.0%	Uranium na	3809.05	22
7	0.1720124E+00003	0.1719697E+00003	0.4269534E-00001	0.2190	0.	4.27E-02	0.0%	0.0%	300 series s	172.012	27
8	0.1044364E+00003	0.1042832E+00003	0.1532335E+00000	0.7859	1.	1.53E-01	0.1%	0.1%	Aluminum	104.436	29
9	0.7343848E+00003	0.7342995E+00003	0.8533886E-00001	0.4377	0.	8.53E-02	0.0%	0.0%	Tin	734.385	30
10	0.7424525E+00004	0.7424570E+00004	-.4510647E-00001	-0.2313	-0.	-4.51E-02	0.0%	0.0%	Molybdenit	7424.53	39
11	0.2980018E+00004	0.2980025E+00004	-.6820319E-00002	-0.0350	-0.	-6.82E-03	0.0%	0.0%	Nickel	2980.02	40
12	0.6190798E+00003	0.6190817E+00003	-.1854778E-00002	-0.0095	-0.	-1.85E-03	0.0%	0.0%	Mischmetal	619.08	42
13	0.1329016E+00003	0.1330059E+00003	-.1043142E+00000	-0.5350	-0	-1.04E-01	-0.1%	0.1%	Magnesium	132.902	43
14	0.1013786E+00003	0.1013490E+00003	0.2963721E-00001	0.1520	0.	2.96E-02	0.0%	0.0%	Silicon carb	101.379	44
Mean =								0.0%			
Std Dev =								0.0%			
Y = 119.933 + 0.997418*C + 0.2280506*E + 0.01569349*R*R + -0.01026542*E*E + 0.003467568*I*I + 0.0168828*A*D + -0.01300526*C*F + 0.09502298*C*J + 0.06335243*D*E + -0.3746707*E*G + -0.1384156*H*L											
From Kriging											
DATA	Y	YHAT	RESIDUAL	StdR		Residual	% error	Absolute value of % error	Material	Y	Data point
1	0.1426823E+00003	0.1405466E+00003	-.2135731E+00001	-0.1872		-2.14E+00	-1.5%	1.5%	AlMg3	142.682	1
2	0.9665366E+00004	0.1255297E+00005	0.2887604E+00004	3.3044		2.89E+03	29.9%	29.9%	Antimony	9665.37	2
3	0.3766261E+00003	0.4220802E+00003	0.4545412E+00002	-0.1297		4.55E+01	12.1%	12.1%	Cobalt	376.626	6
4	0.1021553E+00004	0.1018564E+00004	-.2988678E+00001	-0.1883		-2.99E+00	-0.3%	0.3%	Iron nickel-	1021.55	16
5	0.3149437E+00003	0.3087713E+00003	-.6172373E+00001	-0.1921		-6.17E+00	-2.0%	2.0%	Lead	314.944	18
6	0.3809048E+00004	0.4009645E+00004	0.2005971E+00003	0.0577		2.01E+02	5.3%	5.3%	Uranium na	3809.05	22
7	0.1720124E+00003	0.1800641E+00003	0.8051736E+00001	-0.1749		8.05E+00	4.7%	4.7%	300 series s	172.012	27
8	0.1044364E+00003	0.9666658E+00002	-.7769823E+00001	-0.1940		-7.77E+00	-7.4%	7.4%	Aluminum	104.436	29
9	0.7343848E+00003	0.5985796E+00003	-.1358052E+00003	-0.3487		-1.36E+02	-18.5%	18.5%	Tin	734.385	30
10	0.7424525E+00004	0.6240122E+00004	-.1184403E+00004	-1.6158		-1.18E+03	-16.0%	16.0%	Molybdenit	7424.53	39
11	0.2980018E+00004	0.3317994E+00004	0.3379765E+00003	0.2237		3.38E+02	11.3%	11.3%	Nickel	2980.02	40
12	0.6190798E+00003	0.6153330E+00003	-.3746827E+00001	-0.1892		-3.75E+00	-0.6%	0.6%	Mischmetal	619.08	42
13	0.1329016E+00003	0.1346099E+00003	0.1708327E+00001	-0.1826		1.71E+00	1.3%	1.3%	Magnesium	132.902	43
14	0.1013786E+00003	0.1024939E+00003	0.1115299E+00001	-0.1833		1.12E+00	1.1%	1.1%	Silicon carb	101.379	44
Mean =								8.0%			
Std Dev =								8.7%			

the model, the reliability of the model, and how robust the model is to use for its intended purpose [89,120]. 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

Table 20: Model accuracy after the Maximin Distance sequential infilling sampling

After Infilling with Maximin distance:											
DATA	Y	YHAT	RESIDUAL	StdR	StuR	Residual	% error	Absolute value of % error	Material	Y	Data point
2	0.9665366E+00004	0.9665366E+00004	0.4875838E-00003	0.0047	0.0280	4.88E-04	0.0%	0.0%	Antimony	9665.366	2
39	0.7424525E+00004	0.7424526E+00004	-.1229936E-00002	-0.0118	-0.0701	-1.23E-03	0.0%	0.0%	Molybdenite	7424.525	39
22	0.3809048E+00004	0.3809049E+00004	-.1098495E-00002	-0.0105	-0.0628	-1.10E-03	0.0%	0.0%	Uranium natur	3809.048	22
31	0.1562633E+00004	0.1562632E+00004	0.1437907E-00002	0.0138	0.0697	1.44E-03	0.0%	0.0%	Copper	1562.633	31
18	0.3149437E+00003	0.3149433E+00003	0.4364565E-00003	0.0042	0.0082	4.36E-04	0.0%	0.0%	Lead	314.9437	18
44	0.1013786E+00003	0.1013788E+00003	-.1634298E-00003	-0.0016	-0.0094	-1.63E-04	0.0%	0.0%	Silicon carbide	101.3786	44
40	0.2980018E+00004	0.2980012E+00004	0.6493939E-00002	0.0621	0.3351	6.49E-03	0.0%	0.0%	Nickel	2980.018	40
4	0.2641319E+00004	0.2641306E+00004	0.1277924E-00001	0.1222	0.2796	1.28E-02	0.0%	0.0%	Bronze	2641.319	4
16	0.1021553E+00004	0.1021548E+00004	0.4958011E-00002	0.0474	0.1983	4.96E-03	0.0%	0.0%	Iron nickel-chr	1021.553	16
1	0.1426823E+00003	0.1426811E+00003	0.1235540E-00002	0.0118	0.0698	1.24E-03	0.0%	0.0%	AlMg3	142.6823	1
30	0.7343848E+00003	0.7343912E+00003	-.6440021E-00002	-0.0616	-0.3037	-6.44E-03	0.0%	0.0%	Tin	734.3848	30
42	0.6190798E+00003	0.6190742E+00003	0.5607343E-00002	0.0536	0.2695	5.61E-03	0.0%	0.0%	Mischmetal	619.0798	42
3	0.2077479E+00004	0.2077501E+00004	-.2240740E-00001	-0.2143	-0.4374	-2.24E-02	0.0%	0.0%	Brass	2077.479	33
43	0.1329016E+00003	0.1329001E+00003	0.1537467E-00002	0.0147	0.0879	1.54E-03	0.0%	0.0%	Magnesium-all	132.9016	43
29	0.1044364E+00003	0.1044339E+00003	0.2496074E-00002	0.0239	0.1092	2.50E-03	0.0%	0.0%	Aluminum	104.4364	29
27	0.1720124E+00003	0.1720067E+00003	0.5741325E-00002	0.0549	0.1247	5.74E-03	0.0%	0.0%	300 series stair	172.0124	27
45	0.4809900E+00002	0.4809725E+00002	0.1752324E-00002	0.0168	0.0957	1.75E-03	0.0%	0.0%	Carbon	48.099	45
6	0.3766261E+00003	0.3766118E+00003	0.1431167E-00001	0.1369	0.4675	1.43E-02	0.0%	0.0%	Cobalt	376.6261	6
32	0.3862170E+00003	0.3861905E+00003	0.2654022E-00001	0.2538	0.7547	2.65E-02	0.0%	0.0%	Zinc	386.217	32
23	0.4418757E+00003	0.4419117E+00003	-.3599582E-00001	-0.3442	-0.7628	-3.60E-02	0.0%	0.0%	Titanium zinc p	441.8757	23
28	0.8804123E+00002	0.8805512E+00002	-.1389175E-00001	-0.1329	-0.3083	-1.39E-02	0.0%	0.0%	Cast iron	88.04123	28
11	0.1410945E+00003	0.1411197E+00003	-.2516546E-00001	-0.2407	-0.4475	-2.52E-02	0.0%	0.0%	Ferronickel	141.0945	11
46	0.9448632E+00001	0.9446555E+00001	0.2077061E-00002	0.0199	0.0279	2.08E-03	0.0%	0.0%	Charcoal	9.448632	46
9	0.2508595E+00002	0.2511637E+00002	-.3042402E-00001	-0.2910	-0.4015	-3.04E-02	-0.1%	0.1%	Epoxy resin	25.08595	9
3	0.2156056E+00001	0.2160119E+00001	-.4062730E-00002	-0.0389	-0.0405	-4.06E-03	-0.2%	0.2%	Brick	2.156056	3
19	0.2568233E+00001	0.2552282E+00001	0.1595070E-00001	0.1525	0.1836	1.60E-02	0.6%	0.6%	Limestone	2.568233	19
17	0.1091261E+00001	0.1078484E+00001	0.1277671E-00001	0.1222	0.1313	1.28E-02	1.2%	1.2%	Kiln dried lumb	1.091261	17
37	0.2604455E+00001	0.2635406E+00001	-.3095083E-00001	-0.2960	-0.3549	-3.10E-02	-1.2%	1.2%	HDPE granulat	2.604455	37
68	0.2386153E+00001	0.2336531E+00001	0.4962249E-00001	0.4746	0.5535	4.96E-02	2.1%	2.1%	Clay	2.386153	68
67	0.1898363E+00001	0.1950679E+00001	-.5231564E-00001	-0.5003	-0.5225	-5.23E-02	-2.8%	2.8%	Concrete block	1.898363	67
62	0.4415654E+00001	0.4548318E+00001	-.1326643E+00000	-1.2687	-1.3469	-1.33E-01	-3.0%	3.0%	Polybutadiene	4.415654	62
38	0.1245942E+00001	0.1129600E+00001	0.1163424E+00000	1.1127	1.3871	1.16E-01	9.3%	9.3%	Green veneer p	1.245942	38
71	0.2629080E+00000	0.2891486E+00000	-.2624060E-00001	-0.2510	-0.2738	-2.62E-02	-10.0%	10.0%	Asbestos (with	0.262908	71
70	0.2355338E+00001	0.2087884E+00001	0.2674543E+00000	2.5578	2.7732	2.67E-01	11.4%	11.4%	Scrap iron	2.355338	70
72	0.7569090E+00000	0.8757189E+00000	-.1188099E+00000	-1.1362	-1.2283	-1.19E-01	-15.7%	15.7%	Cold rolled she	0.756909	72
7	0.5979600E-00001	0.1079745E+00000	-.4817851E-00001	-0.4608	-0.5010	-4.82E-02	-80.6%	80.6%	Corrugated bo	0.059796	7
								Mean =	3.8%		
								Std Dev =	13.7%		
$Y = 0.05860287 + 1.237871 * R + 1.056571 * A + 1.008596 * C + 0.7801412 * D + 1.089715 * E + 0.9841712 * F + 0.6166319 * G + 2.383661 * H + 0.7763125 * L + 0.004913406 * R * R + 8.989214E-07 * C * C + 0.007313005 * E * E + 0.02540538 * G * G + 0.01208991 * I * I + 0.1854093 * L * L + 0.007325138 * R * D + 0.02496565 * R * H + 0.05660541 * R * L + 0.002324183 * B * C + 0.000155864 * C * G + 0.2967796 * E * K + 0.4580382 * E * L + 0.0291983 * F * J$											

Table 21: Model predictability and robustness test

Yhat PR model	Residual	% error	Absolute value of % error	Material	Y	Data point	Yhat Kriging	Residual Kriging	% error Kriging	Absolute value of % error Kriging
21.0253	3.19216	13.2%	13.2%	Ceramics	24.22	5	17.8533173	6.364192698	26.3%	26.3%
1.64257	0.09908	5.7%	5.7%	Dry veneer plywood	1.742	8	1.140857152	0.600796848	34.5%	34.5%
6.36742	-0.2199	-3.6%	3.6%	EPS	6.147	10	9.730113232	-3.58262023	-58.3%	58.3%
7.35121	0.25672	3.4%	3.4%	Glass	7.608	12	7.895543052	-0.28761605	-3.8%	3.8%
2.52608	-0.3204	-14.5%	14.5%	Graphite	2.206	13	7.136587987	-4.93089999	-223.6%	223.6%
6.80192	-0.3961	-6.2%	6.2%	HDPE	6.406	14	35.96002349	-29.5541875	-461.4%	461.4%
8.27397	-2.1456	-35.0%	35.0%	HIPS	6.128	15	21.20274975	-15.0743538	-246.0%	246.0%
128.101	0.95016	0.7%	0.7%	Magnesium	129.1	20	138.6348067	-9.58330674	-7.4%	7.4%
26.034	1.29545	4.7%	4.7%	Zinc Oxide	27.33	21	39.81150675	-12.4820667	-45.7%	45.7%
10.3047	2.77498	21.2%	21.2%	Synthetic rubber	13.08	24	10.81536559	2.264294406	17.3%	17.3%
34.181	-0.2557	-0.8%	0.8%	Silicone	33.93	25	19.36287919	14.56235081	42.9%	42.9%
80.3126	-2.3442	-3.0%	3.0%	Low alloy steel	77.97	26	74.90995175	3.058478252	3.9%	3.9%
13.8747	-1.609	-13.1%	13.1%	Nylon 6	12.27	34	14.68323896	-2.41755896	-19.7%	19.7%
6.71235	0.11133	1.6%	1.6%	Oriented strand board	6.824	35	14.44927275	-7.62559975	-111.8%	111.8%
8.29699	-0.6061	-7.9%	7.9%	PVC	7.691	36	9.185320242	-1.49444424	-19.4%	19.4%
60.5247	-0.331	-0.5%	0.5%	Lithium	60.19	41	33.87467147	26.31904853	43.7%	43.7%
38.6013	-1.9587	-5.3%	5.3%	Polyester resin glass fiber	36.64	47	68.49923885	-31.8566689	-86.9%	86.9%
19.7913	5.24172	20.9%	20.9%	MG-silicone	25.03	48	15.87687217	9.156187828	36.6%	36.6%
17.3331	-2.2138	-14.6%	14.6%	Polycarbonate	15.12	49	20.49418917	-5.37485917	-35.5%	35.5%
48.324	-2.9906	-6.6%	6.6%	Ferrochromium	45.33	50	72.07067265	-26.7373326	-59.0%	59.0%
13.7786	-0.91	-7.1%	7.1%	Nylon 66	12.87	51	22.89303594	-10.0244359	-77.9%	77.9%
13.6577	-0.8504	-6.6%	6.6%	Nylon 6 glass filled	12.81	52	27.72709295	-14.919813	-116.5%	116.5%
4.51	-0.2863	-6.8%	6.8%	Polyurethane rigid foam	4.224	53	3.695899812	0.527824188	12.5%	12.5%
21.9634	0.37598	1.7%	1.7%	Glass fiber	22.34	54	23.76224165	-1.42287165	-6.4%	6.4%
12.5796	-0.9494	-8.2%	8.2%	Nylon 66 glass filled	11.63	55	26.63915301	-15.008993	-129.1%	129.1%
6.56019	-0.089	-1.4%	1.4%	Polypropylene	6.471	56	27.97504616	-21.5038942	-332.3%	332.3%
6.52119	-0.5812	-9.8%	9.8%	Low Density Polyethylene	5.94	57	27.78263929	-21.8426163	-367.7%	367.7%
24.3	2.69254	10.0%	10.0%	Ferrite	26.99	58	29.76028209	-2.76774209	-10.3%	10.3%
36.6571	2.36725	6.1%	6.1%	Ferromanganese	39.02	59	41.35665996	-2.33233996	-6.0%	6.0%
24.7372	0.42559	1.7%	1.7%	Magnetite	25.16	60	24.92253387	0.240206126	1.0%	1.0%
3.99239	-0.0847	-2.2%	2.2%	Polystyrene GPPS	3.908	61	5.803894098	-1.8961841	-48.5%	48.5%
30.5089	4.90078	13.8%	13.8%	Pig iron	35.41	63	55.53288585	-20.1232058	-56.8%	56.8%
39.7899	0.56287	1.4%	1.4%	Cadmium	40.35	64	45.32173314	-4.96899314	-12.3%	12.3%
2.62116	0.39422	13.1%	13.1%	Laminated veneer lumber	3.015	65	5.243689312	-2.22830831	-73.9%	73.9%
1.75393	0.16692	8.7%	8.7%	Plywood	1.921	66	1.713999966	0.206851034	10.8%	10.8%
2.02638	-0.1937	-10.6%	10.6%	Bauxite	1.833	69	6.280770391	-4.44812939	-242.7%	242.7%
		Mean =	8.1%						Mean =	85.8%
		Std Dev =	7.2%						Std Dev =	113.3%
				Model Accuracy:	Mean =	3.8%			Std Dev	13.7%
				Model Reliability:	Mean =	8.1%			Std Dev	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.				

variability due to the accuracy and reliability measures. The following subsections illustrate all three evaluations by following the same example introduced in the prior two subsections. Testing

this example could be advantageous, because if a model is valid for a diverse array of materials based on total environmental impact per unit volume, such an approach could be promising for design problems that compare sets of composites and components by transformation of the data set using Equation (10).

7.4.3.1. Model accuracy

Table 19 shows the comparative results of modeling with both second order polynomial regression and Kriging method from the original data set of fourteen points identified by the Latin Hypercube method. The average absolute error measure here also shows that the second order polynomial regression is more accurate in this case. Also, a polynomial function is identified by the regression method to clearly define the surrogate model. Table 20 shows the resulting model and accuracy measure for the complete set of thirty-six data points identified after the Maximin Distance sequential infilling sampling process. Both the mean and standard deviations were calculated for the absolute error measures. The average absolute error (AAE) and its sample standard deviation (S) were computed by the following two formulas.

$$AAE = \frac{1}{m} \sum_{i=1}^m |y_i - \hat{y}_i| = \bar{X} \quad (11)$$

$$S = \sqrt{\frac{\sum_{i=1}^m (x_i - \bar{x})^2}{m-1}} \quad (12)$$

7.4.3.2. Model reliability

Table 21 shows the actual and predicted values of the remaining thirty-six materials that are not included in the constructed model. Predicted values, labeled 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 and not the Kriging model

due to significant difference in model accuracy for this example. The statistical information about the model accuracy and reliability along with the resolution in the design space are all useful to evaluate the model robustness. The next subsection highlights an evaluation approach.

7.4.3.3. Model uncertainty and robustness

Approaches were used to measure model robustness in a prior study [122]. Some variability inherently exists in an approximate model, as the previous subsections demonstrate. A model is robust only if the variability does not prevent the selection of an acceptable design alternative. Thus, a high fidelity model is not necessary if an approximate model constructed from known data is robust enough to select an alternative that is close enough to the optimal solution [82,83]. 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.

The derivation of the expressions used to determine model robustness is as follows. Given that event A is unacceptable model accuracy and event B is unacceptable model reliability, events A and B are then statistically independent because any data point is either in the sample set to test model accuracy or not in the sample set to test model reliability. No point, x, which is expressed as average absolute error, can test for both events A and B. Thus probabilistically,

$$P(x(A) \text{ and } x(B)) = P(x(A)) P(x(B)) \quad (13)$$

Here it is assumed that for a large enough sample size, n,

$$\bar{X} \approx \mu \quad (14)$$

$$S \approx \sigma \quad (15)$$

Where a normal distribution of the data is assumed Z is the critical value for the normal distribution, where

$$Z = \frac{x - \mu}{\sigma} \approx \frac{x - \bar{X}}{S} \quad (16)$$

If it is assumed that the acceptable limit for both model accuracy and reliability are both one standard deviation above the mean, from any cumulative standardized normal distribution table:

$$P(x = x_{ul}(A)) = P(Z(A) = 1) = P(x = x_{ul}(B)) = P(Z(B) = 1) = 0.8413 \quad (17)$$

$$1 - P(Z = 1) = 0.1587 \quad (18)$$

$$P(x_{ul}(A) \text{ and } x_{ul}(B)) = 0.1587^2 = 0.0252 \quad (19)$$

Where,

$$x_{ul}(A) = \mu_A + \sigma_A \quad (20)$$

$$P(x = x_{ul}(A)) = P(Z(A) = 1) = P(\mu_A + \sigma_A) \quad (21)$$

$$x_{ul}(B) = \mu_B + \sigma_B \quad (22)$$

$$P(x = x_{ul}(B)) = P(Z(B) = 1) = P(\mu_B + \sigma_B) \quad (23)$$

For $x_{ul}(A)$ and $x_{ul}(B)$ to both occur simultaneously at both limits where by previous definition,

$$x_{A \text{ and } B \text{ error}} = \mu_A + \sigma_A + \mu_B + \sigma_B \quad (24)$$

Equation (24) computes the actual total error value at this suggested limit and equation (19) computes the probability of occurrence of this suggested limit. Equation (19) shows that the probability is 2.52% that this will happen, or 97.48% that this will not happen.

Between alternatives in a data set,

$$Resolution_{avg} = \frac{x_{max} - x_{min}}{(n-1)x_{avg}} \quad (25)$$

where n is the total sample size.

The expected average number of alternatives displaced from the best alternative by using this model with 97.48% confidence on average is:

$$\# \text{ of alternatives displaced}_{avg} = \frac{x_{A \text{ and } B \text{ error}}}{Resolution_{avg}} \quad (26)$$

For the example shown in Tables 20 and 21, 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 seventy-two different alternatives and calculate the average difference in the values between each of the adjacent pairs of alternatives. For the example shown in Tables 20 and 21, this average percentage difference 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. In other words, it is very likely that an alternative in the top three of the seventy-two material alternatives would be selected by using this model. If that expectation is acceptable to the designer, this surrogate model could be used. The following section describes how these models might be used in a design process.

7.5. Selection of the Optimal Design Concept

A specific problem should first be formulated. Equation (10) provided a way to convert standard data into problem specific data sets from any information provided by a designer about a problem. Here, the generation of a data set for the environmental attribute is computed directly from Equation (10). Masses of the components can be computed by simply multiplying the part volumes and the material mass densities. The masses will also be 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. It is recommended

to construct models for each of these single attributes separately at first based on the utility values of the attribute. This is explained in the following subsection.

7.5.1. Single attribute optimization

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 [107]. Thus, it is important to optimize each attribute's utility model individually to observe the effect of all known and potential dependent variables. A check of the linear correlation coefficient between variables and attributes could reveal dependencies. It is recommended to include any variables that an attribute may depend upon in the model to best observe relationships in a design situation accurately [124]. A utility function can introduce some additional nonlinear effects beyond any that exist in a function of the attribute values as examples in a prior work indicated [107]. Model accuracy and reliability could be lessened some in extreme locations of the design space that are far away from data locations used to construct and test the model due to the lack of ordered and balanced data locations for material selection. All single attribute models should be compared side by side at the same optimal data point locations to construct or visualize the Pareto optimal frontier [107] for the next step covered in the following subsection.

7.5.2. Optimization of multiple attributes

Section 7.2.3.1 briefly discussed preference modeling methods that can identify a specific optimal point on a Pareto optimal curve. The multi-attribute utility (MAU) function is a composite linear combination of the single attribute values and their preference weights [125]. 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 single attribute utility 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 optimization with surrogate models by clustering to find more accurate points in the optimal regions of interest [123]. However, the optimal solution may not be located at a data point where a known material exists. Thus, it is recommended to check the Euclidean distance between the optimal point or points and the known data points. This would 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 realized. That would require a search for a similar material or materials with the better properties, but this process would alert the designer to any better potential possibilities.

7.5.3. Feasible region to comply with regulations

Many traditional design optimization 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 [51]. A key issue concerns the degree to which such information can be represented as constraints in a constrained optimization mathematical formulation. That would depend upon the mathematical alignment of a given standard with an LCA computational structure. Thus, it is recommended to include standards as mathematical limits in a constrained optimization 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. The next section demonstrates the application of the entire methodology in a practical example design problem.

7.6. Case Study: Automobile Disc Brake

The following four subsections highlight the use of the new MASSDOP method in an example of a design solution that is more capable as a result of the MASSDOP method

deployment. This case study problem is the same example as the one used in the previous chapter to demonstrate an information modeling methodology [51].

7.6.1. Background of Problem

Common performance objectives for the design of a set of rotor and caliper pads include minimization of the vehicle stopping distance, minimization 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 degrees C. Results for specific design alternatives were calculated by using the conventional engineering formulations [71]. Some information was obtained to estimate the specific values of rotor material property parameters [72]. 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 does show simultaneous consideration of performance, environmental, and economic objectives. However, this example is not a multi-objective problem in that it lacks tradeoffs among the various objectives. Such a situation can occur in actual design applications. In this case, objectives such as minimizing vehicle stopping distance, maximizing heat dissipation, and minimizing wear mass all depend predominantly upon different design variables. Due to the large number of design variables in this problem, variables common to all objectives such as mass density or initial thickness do not have a consistent linear correlation among design alternatives. Thus, a change in such a common design variable value does not necessarily cause one objective to improve while another worsens in this example. Nevertheless, the following subsections illustrate the efficient and effective use of the new MASSDOP method to formulate the solution of this problem.

7.6.2. Problem Formulation

To simplify the illustration, a single performance objective of minimizing vehicle stopping distance was used. That objective depends only upon the coefficient of friction between the rotor and pad materials based on assumptions of reasonable operating conditions. From there, adequate heat dissipation could be considered an additional constraint. The initial minimum solid volume of the rotor and pads can simply be computed for each material combination alternative at the given constraint values. For this example, the solid volume of the pad is proportional to the pads' initial thickness due to constant area, and the rotor's solid volume is a function of the initial rotor thickness and the solid volume percentage. Rotors are usually casted to a hollowed shape to add a convection cooling feature. Life cycle assessment and life cycle costing formulations indicate that minimization of mass for a given material would directly help to optimize both of those objectives.

Table 22 shows the main specific alternatives identified by prior work [72] along with pad alternatives found from general searches as used in an example in prior work [51]. Six different possible rotor materials are labeled "A" through "F", and eleven different potential pad materials are labeled "1" through "11". Every possible material combination is labeled 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 22 are a concern based on regulations of copper content in two states [126,127].

Some of the combinations were found to be infeasible for the given temperature limit and heat dissipation and life requirements. Thus, there are a total of forty-six alternatives of material combinations in the original design set [51]. From the derived information, 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 (10). Volume data was converted to mass for each alternative to generate the data set for the life

cycle cost attribute. Additional data of molded 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.

Table 22: Matrix of material combination alternatives [51]

		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) fibers	A3	B3	C3	D3	E3	F3
	aramid Nomex fibers	A4	B4	C4	D4	E4	F4
	Kevlar fibers	A5	B5	C5	D5	E5	F5
	Twaron fibers	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 fibers	A10	B10	C10	D10	E10	F10
	other plastics	A11	B11	C11	D11	E11	F11

Concern of greater than 0.5% Copper content

7.6.3. 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 multi-attribute utility (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 an entire 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 labeled as “u” followed by an attribute subscript number and the MAU variable is labeled as “U”. For this example, it was assumed that a designer’s preference is represented by the vector of preference weights previously assumed [111] of {0.214,0.429,0.357} with a first attribute of performance, second attribute of cost, and third of environmental impact.

Table 23: Results from testing the constructed surrogate model for multiple attribute utility (MAU) values

Polynomial Regression had an R-Sq(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*Disk mass in kg*J + -0.0003781217*Pads cost in USD/kg includes molding*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

DATA	Y	YHAT	RESIDUAL	StdR	StuR	Residual	% error	Absolute value of % error	Alternative #	Y	Data point
1	0.8970000E+00000	0.8971903E+00000	-.1903208E-00003	-0.2888	-0.3561	-1.90E-04	0.0%	0.0%	A1	0.897	1
4	0.8220000E+00000	0.8234002E+00000	-.1400155E-00002	-2.1248	-2.2969	-1.40E-03	-0.2%	0.2%	A4	0.822	4
5	0.8310000E+00000	0.8303853E+00000	0.6146645E-00003	0.9328	1.0828	6.15E-04	0.1%	0.1%	A5	0.831	5
6	0.8240000E+00000	0.8241103E+00000	-.1102651E-00003	-0.1673	-0.1810	-1.10E-04	0.0%	0.0%	A6	0.824	6
7	0.8250000E+00000	0.8241691E+00000	0.8309013E-00003	1.2609	1.3699	8.31E-04	0.1%	0.1%	A7	0.825	7
8	0.8860000E+00000	0.8857044E+00000	0.2956058E-00003	0.4486	0.9158	2.96E-04	0.0%	0.0%	A8	0.886	8
11	0.8210000E+00000	0.8210933E+00000	-.9332981E-00004	-0.1416	-0.1717	-9.33E-05	0.0%	0.0%	A11	0.821	11
15	0.3600000E+00000	0.3601409E+00000	-.1409355E-00003	-0.2139	-0.3538	-1.41E-04	0.0%	0.0%	C5	0.360	15
16	0.3620000E+00000	0.3616421E+00000	0.3579375E-00003	0.5432	0.6654	3.58E-04	0.1%	0.1%	C6	0.362	16
17	0.3630000E+00000	0.3632000E+00000	-.2000006E-00003	-0.3035	-0.4093	-2.00E-04	-0.1%	0.1%	C7	0.363	17
22	0.5480000E+00000	0.5477250E+00000	0.2750279E-00003	0.4174	0.7689	2.75E-04	0.1%	0.1%	D1	0.548	22
25	0.5950000E+00000	0.5957393E+00000	-.7392883E-00003	-1.1219	-1.3667	-7.39E-04	-0.1%	0.1%	D4	0.595	25
26	0.6640000E+00000	0.6632244E+00000	0.7755660E-00003	1.1770	1.4048	7.76E-04	0.1%	0.1%	D5	0.664	26
27	0.5970000E+00000	0.5969606E+00000	0.3935637E-00004	0.0597	0.0736	3.94E-05	0.0%	0.0%	D6	0.597	27
29	0.6940000E+00000	0.6941293E+00000	-.1292781E-00003	-0.1962	-0.4052	-1.29E-04	0.0%	0.0%	D8	0.694	29
30	0.6240000E+00000	0.6239909E+00000	0.9066528E-00005	0.0138	0.0451	9.07E-06	0.0%	0.0%	D9	0.624	30
31	0.6490000E+00000	0.6491113E+00000	-.1113232E-00003	-0.1689	-0.4512	-1.11E-04	0.0%	0.0%	D10	0.649	31
33	0.7380000E+00000	0.7381526E+00000	-.1525629E-00003	-0.2315	-0.4825	-1.53E-04	0.0%	0.0%	E1	0.738	33
34	0.6370000E+00000	0.6370919E+00000	-.9186573E-00004	-0.1394	-0.1838	-9.19E-05	0.0%	0.0%	E2	0.637	34
35	0.7060000E+00000	0.7058911E+00000	0.1088663E-00003	0.1652	0.2535	1.09E-04	0.0%	0.0%	E3	0.706	35
36	0.6100000E+00000	0.6097384E+00000	0.2616396E-00003	0.3971	0.5476	2.62E-04	0.0%	0.0%	E4	0.610	36
38	0.6130000E+00000	0.6132208E+00000	-.2208171E-00003	-0.3351	-0.3882	-2.21E-04	0.0%	0.0%	E6	0.613	38
42	0.5640000E+00000	0.5639885E+00000	0.1151016E-00004	0.0175	0.0354	1.15E-05	0.0%	0.0%	E10	0.564	42
Mean = 0.0%											
Std Dev = 0.0%											

For the data points not included in the PR model:

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

Table 23 shows the surrogate model constructed for this specific design example by applying the methods introduced in Section 5. Here, it is evident that the Latin Hypercube space filling followed by the Maximin Distance sequential infilling resulted in a model accuracy with negligible error. The bottom portion of Table 23 illustrates the test for model predictability by comparison of actual responses to those predicted by the model constructed by the sampling stages. These results show a significant difference between the model reliability predicted by all data points and that predicted when only those points in the neighborhood 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 can be ignored, 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.

7.6.4. Search for the Optimal Solution in an Entire Design Space

In the prior subsection, the expected differences between actual and predicted MAU values in an alternative set were investigated. Figure 24 shows the actual utility values of each single attribute and of the composite multi-attribute utility plotted by the bottom four curves in the legend. Section 7.5 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 24, poses some challenges with finding a single optimum point. In this case, the genetic algorithm was used to search globally for potential optimal solutions. Several hundred of the final iterations identified predicted MAU values over 0.95.

As Section 7.5.2 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 as possible. In Figure 24, the corresponding alternatives are shown on the horizontal axis from left to right ordered by shortest Euclidean distance to a predicted target optimal point. Section 7.5 warns of the potential accuracy issue with predicted optimal points on the outskirts of a design space away from the limited design set of discrete material-related data locations that were available to construct the surrogate model. Thus, Figure 24 shows a significant difference between the actual and predicted MAU values of the

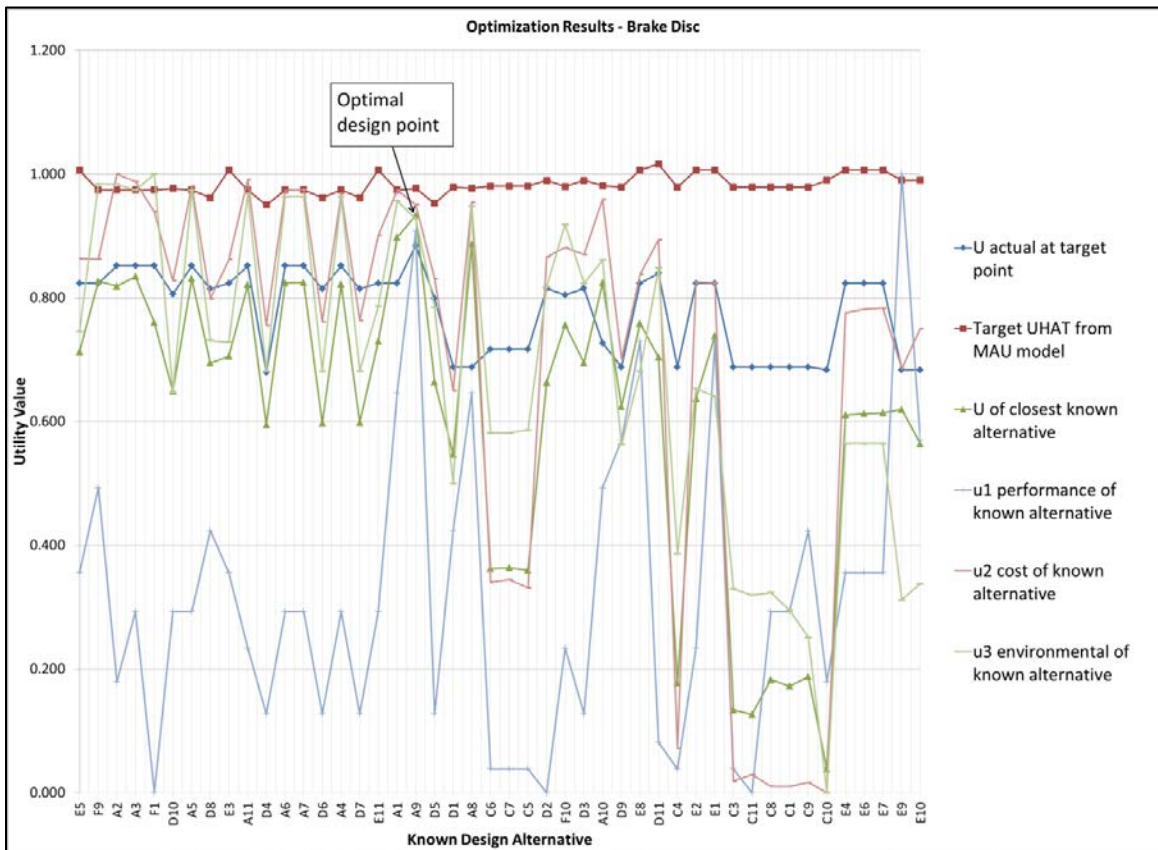


Figure 24: Results from optimization of a brake disc design

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 24 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 modeling 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 [51] and after this new MASSDOP method was developed. In addition to a view of the entire design space not previously realized, the design process with MASSDOP took only about 25% of the time to execute compared to a prior less efficient method of modeling a complete Life Cycle Assessment for every design alternative. The new MASSDOP method as deployed in this example could be extendable to other practical engineering design problems.

7.7. MASSDOP Discussion

This work addressed several main objectives. First, the investigation concerned the efficient and effective integration of credible Life Cycle Assessment (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 an entire design space beyond a mere set of known design alternatives. Third, the construction of usable surrogate models for material selection involves the additional challenge of using data points in the design space that are not in desirable locations for traditional design space filling sampling techniques. Fourth, it was necessary to demonstrate the effective and efficient deployment of the new 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 [34,91,92], 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. That approach was described in Section 7.1.

Investigation indicated that material selection is 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 7.2 covered the rationale for a foundation of the methodical approach described in Section 7.3 to address this issue.

Section 7.3 also prescribed a technique to map input parameters to output responses that is essential for surrogate model construction as described in Section 7.4. The use of approximate, or surrogate, modeling can be ideal to efficiently streamline the complex computational structure of both Life Cycle Assessment (LCA) and traditional physics-based formulations of predictive product performance. Section 7.3 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 minimizing cost and environmental impact and maximizing performance objectives. Although the case study presented here does not happen to exhibit such tradeoffs, it does provide a useful demonstration of how the new 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. The second important topic area that could benefit from further research concerns the representation of parametric uncertainty. Although only mean values of all parameters were presented in this work, prior work demonstrated that consideration of uncertainty can influence the selected design concept [46].

One of the key contributions of this work was the development of a method to construct surrogate models that can consider all objectives in the decision model efficiently and effectively for concept selection. Section 7.4 described this new method in depth. This development included the investigation of possible space filling sampling (SFS) and sequential infilling sampling (SIS) two stage approaches to adapt and deploy in ways that address the unique challenges of material selection. Useful examples were presented in both Section 7.4 and Section 7.6, 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. Section 7.5 explained how usable models of an entire 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 7.6. 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 in effective concept selection in some cases.

CHAPTER 8

CONCLUSIONS

The overall goal of this dissertation was to address three main barriers to the design of products for sustainability that the prior works had not been able to resolve. First, Life Cycle Assessment (LCA) models in their current forms that conform to ISO 14040-14044 are not suited to early design due to complexity, too many variables, and the lack of holistic consideration of cost and other criteria over a product's life cycle. This work addressed that challenge by the unique contribution of a normative decision analysis-based formulation to accurately account for all significant input flows. Salient features of this approach include a systematic representation to propagate uncertainties, as well as a preference based multi-attribute modeling to simultaneously account for a product's performance along with environmental and cost impacts over the product's life cycle. Second, standards information related to compliance is not well aligned with information about environmental impacts as predicted by LCA to facilitate decision making during early design stages. That research challenge was addressed by the salient features of a novel ontological framework that: represents both the objectives that pertain to sustainable design and the applicable sustainability standards and regulations, and integrates different domains of information by the semantic relationships between taxonomies to enable decision making informed in real time. Third, material selection is both a significant factor in sustainable design and also not conducive to more efficient and robust surrogate model construction due to the inflexible discrete locations of material related data points and the dimensionality of the data. This difficult research challenge was resolved by the combination of several new salient features. Manageable dimensionality of LCA was achieved with a minimal loss of the important information by the consolidation of significant factors into categorized groups. A streamlined process that avoids the construction of full LCA facilitates enhanced efficiency. A unique formulation was developed to combine efficiency of use with a mathematically rigorous representation of any pertinent objectives across an entire design space. In order to resolve the

important issue of robust surrogate model construction for material selection, an adapted two stage sampling approach was introduced based on a feasible approximation of a Latin Hypercube design at the first stage.

The development of these salient features revealed a number of important outcomes. First, the NASDOP method for normative decision analysis, detailed in Chapter 5, provides the foundation on which all methods were developed. The contributions of NASDOP include several more specific salient features. The capabilities of LCA are concisely defined to accurately represent the material and energy flows and their resulting set of environmental impacts or attributes. Expressions were derived to formulate the associated cost flows for the same set of processes over the complete life cycle of a product unit. Thus, the normative approach allowed consistent modeling of environmental and economic attributes in an accurate mathematical representation. Such an approach was previously shown to facilitate problem formulation at the conceptual design stages for traditional engineering problems. Chapter 5 shows the potential for similar applicability when all sustainability criteria are considered. All attributes in these relationships depend upon parametric data of the associated material flows, substance emissions, or cost flows. This data is available from published sources of information, but has significant uncertainty. Thus, the method to account for all parametric data included a reasonable approach to account for the uncertainty of all significant data sources. The normative formulation included the deployment of hypothetical equivalents and inequivalents method (HEIM) to model the preferences of a designer consistently in a multi-criteria decision making (MCDM) formulation.

This formulation enables the direct comparison of numerous strategic alternatives at the early stages of conceptual design from the design for sustainability perspective. The limitations of a method that only identifies a best potential strategic direction are addressed by the work in Chapter 7. However, such an approach can be very useful for many practical examples such as a redesign for the next generation of a mature and well defined product design. Here, an informed strategic direction could be established at the early stages of redesign. More specific details can

evolve as the design process progresses to inform subsequent design iterations. Since a design process generates information, some information model is needed to represent the pertinent knowledge in some organized fashion. This is especially important when the knowledge related to decisions that must be made is complex. Thus, it is important to capture and communicate the design knowledge on which these decisions about the design direction are based. The work in Chapter 6 provides such an approach along with the needed ontological framework.

The work described in Chapter 6 addresses the need to model the design for sustainability related information and rationale transparently for distributed design based on the context and meaning of the design knowledge. Since information related to compliance with standards and regulations is often decoupled from the information related to environmental objectives as prescribed by LCA, an interoperable ontological framework for engineering design and decision-based design was extended to include the domains of standards and LCA, as represented by NASDOP. Here, these different domains of sustainable design knowledge are linked by the relationships between objects in the different domains. Since the applicable standards and criteria are populated within the same information model in real time, the standards may be adopted more easily early on while the design may also be influenced more toward the triple bottom line objectives of preserving the environment, economic gains, and the interests of affected stakeholders in society. Due to the resulting parallel inspection capabilities to compare information from LCA instances along with the standards as represented by constraints to that of associated specific design alternatives, the resulting information model for the case studied revealed some interesting correlations between standards related measures and the corresponding measures related to environmental objectives in that example. The extent to which such constraints can be included in a mathematical model is examined more closely in Chapter 7. Those results show that such capability depends upon the degree of alignment between standards and impacts as predicted by LCA. The example studied could only model constraints as red flagged alternatives in the data set shown. If the standard applied to its actual intent of limiting

copper emissions to water instead of to the percentage of copper content in the components, then such a constraint might actually be modeled in constrained mathematical optimization expressions. The approach shown in Chapters 6 and 7 illustrates how the information modeling can at least reveal these constraints in real time despite any such disconnects between standards and LCA.

In Chapter 7, the method was introduced to consider all design alternatives of components throughout an entire design space to enable optimal concept selection beyond a limited set of predefined alternatives. Here, the approach focused on material selection due to the significance of that factor from both the sustainability and product performance perspectives. A technique was developed to both streamline the Life Cycle Assessment (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 novel feasible approximation sampling approach addressed the unique challenges posed by rigid data locations of material parameters. Robust results were achieved by use of the adapted Latin Hypercube approach at the first of two sampling stages. The case study example could be designed for sustainability in about one quarter of the time compared to the prior approach of setting up complete LCA models for each design alternative. Furthermore, the same design alternative was selected with either approach, which suggests that the more efficient surrogate modeling approach could be just as effective in similar instances.

8.1. Future Work

Future work could advance and build on this work in several important ways. Chapter 5 revealed the significance of parametric uncertainty in concept selection. More accurate and efficient methods need to be developed to account for these uncertainties in the MASSDOP formulations. Here, expected utility functions could replace mean values if the associated

calculations can be done efficiently enough. Another area pertains to a more diverse selection of case study examples to illustrate the application of MASSDOP. While the brake disc example shows great promise for practical use of the method, that example does not have tradeoffs between the different objectives to illustrate the application in a multi-criteria decision making (MCDM) problem. More examples could better illustrate tradeoffs between environmental, performance, and economic objectives and the importance of modeling the preferences among these often conflicting objectives. The information related to such decisions in these future examples could also be entered as new design instances in the ontological framework that was presented in Chapter 6 to show how related information is captured and communicated early in a distributed design situation. This may also reveal ways that the ontological framework could be modified or extended to maximize the effectiveness in all scenarios. Capstone design projects at universities provide such opportunities. The capabilities of semantic searching for information and the use of reasoning and rules could be utilized to further support decision making in some cases.

In support of examples that best illustrate multi-objective problems, methods are needed for the efficient and effective aggregation of multiple attributes within each objective. Chapter 7 explained how this needs to be addressed in the situation of numerous environmental impacts to consider. This could also be an important issue in some cases that may have multiple performance or economic objectives. Finally, the accuracy, predictability, and robustness of surrogate models depend upon statistics. Chapter 7 showed two example surrogate models with favorable robustness that have a sufficiently large number of data points, or sample size. This is an efficiency issue common to the selection of data sets. It is possible to have not enough data to construct a robust surrogate model, but it is also possible to sacrifice efficiency sought by the use of surrogate modeling if the sample size is too large. Dimensionality and the correlation of variables to responses can affect the optimal sample size of a given problem. Further research in this area should help MASSDOP to be used optimally. Overall, an ideal goal may be to achieve

enough efficiency to mitigate the time invested in using these methods to justify the benefits of more sustainable designs in as many cases as possible.

APPENDIX

DATA TABLE FOR CHARCOAL GRILL CASE STUDY

Table A.1: Calculation results from LCA and LCC

Design Alternatives	GHG	Acidification	Eutrophication	Photochemical	Coal	Crude oil	Iron	Natural gas	Cost																				
	f1	f2	f3	Ozone formation f4	f5	f6	f7	f8	f9																				
	kg CO2 eq	kg SO2 eq	kg NO2 eq	kg CH4 eq	kg eq	kg eq	kg eq	kg eq	USD																				
Baseline mean values	958 1507 2382	345 461 605	0.83 1.38 2.14	0.27 1.17 3.81	2.0 3.9 6.9	1.06 2.04 3.56	1.23 3.89 7.6	5.4 10.3 18.0	70 246 743																				
X1 - Weight reduction	845 1403 2065	3.21 4.43 5.62	0.73 1.28 1.89	0.26 1.15 3.76	2.0 3.9 6.6	0.91 1.87 3.04	0.68 3.32 5.8	4.1 9.0 13.7	69 240 724																				
X2 - Recycled material	958 1500 2382	3.45 4.59 6.05	0.83 1.36 2.14	0.27 1.17 3.81	2.0 3.9 6.9	1.06 2.04 3.56	1.23 3.45 7.6	5.4 10.3 18.0	50 225 722																				
X3 - Reduced energy content	910 1424 2245	3.35 4.47 5.88	0.79 1.32 2.05	0.26 1.16 3.79	2.0 3.9 6.8	1.00 1.92 3.35	0.99 3.43 6.8	4.8 9.2 16.1	65 232 702																				
X4 - Low toxicity	920 1458 2315	3.21 4.29 5.62	0.74 1.23 1.91	0.26 1.14 3.76	2.0 3.9 6.9	1.06 2.04 3.56	1.23 3.89 7.6	5.4 10.3 18.0	70 246 743																				
X5 - Renewable resources	800 1207 1861	3.43 4.59 6.04	0.81 1.37 2.14	0.27 1.17 3.81	1.0 2.0 3.4	0.53 1.02 1.78	0.33 1.78 3.7	2.7 5.2 9.0	58 233 730																				
X6 - Efficient Use	845 1348 2141	2.85 3.82 5.04	0.74 1.23 1.92	0.22 0.91 2.93	1.6 3.1 5.5	0.98 1.88 3.28	1.25 3.93 7.7	5.5 10.5 18.4	57 207 632																				
X7 - Sustainable manufacturing	957 1506 2380	3.44 4.60 6.04	0.83 1.37 2.14	0.27 1.17 3.81	2.0 3.9 6.9	1.06 2.04 3.56	1.23 3.89 7.6	5.4 10.3 18.0	66 234 710																				
Expected range for alternatives given uncertainty	800	1419	2382	2.85	4.43	6.05	0.73	1.32	2.14	0.22	1.13	3.81	1.0	3.6	6.9	0.53	1.86	3.56	0.33	3.45	7.7	2.7	9.4	18.4	50	233	743		
	Low	Mean	High	Low	Mean	High	Low	Mean	High	Low	Mean	High	Low	Mean	High	Low	Mean	High	Low	Mean	High	Low	Mean	High	Low	Mean	High	Low	Mean

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