An Exploration of Materials Taxonomies to Support Streamlined Life Cycle Assessment

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Abstract

As life cycle assessment (LCA) gains prominence as a reliable method of environmental evaluation, concerns about data availability and quality have become more important. LCA is a resource intensive methodology, and thus data gaps pose a frequent challenge, motivating the need for robust streamlining approaches. Existing methods for filling data gaps often ignore the effects of the uncertainty inherent in estimated data. Under-specification, or using structured data to provide less information in product characterization, is one option to incorporate uncertainty, and has been shown to be a viable method both for streamlining and decision-making under uncertainty. However, previous work did not emphasize developing robust data structures intended to balance trade-offs between effectiveness and efficiency in streamlining methods. Furthermore, there was little consideration given to analyzing the environmental profile (multiple impacts) of a process, rather than a single impact.

This thesis explores how data mining techniques can be used to quantitatively develop data structures to enable streamlined assessment. The use of clustering and principal component analysis is explored in an effort to identify potential material classifications, and other statistical methods further assess the classifications. These insights are used to create hierarchical taxonomies that are evaluated in terms of effectiveness and efficiency. The method is applied to life cycle inventory process datasets for three material types (metals, polymers, and precious metals). Four environmental midpoints from the TRACI 2.0 impact assessment method are used to illustrate the uncertainty reduction enabled by classification.

It was found that the most useful classification method for both metals and polymers was based on price, and for precious metals, material type and recycled content. In general, the method was able to select efficient groupings that accounted for a large percentage of the overall variation in the data. With one additional level in the taxonomy, the overall median percent error rates were approximately 30-40% for all impacts except non carcinogenicity, which was 65-80%. This is compared to initial error rates that were on average twice as high for the metals and precious metals datasets. Case studies demonstrated how the analysis and structure provided by this methodology can be useful in comparative decision-making, to reduce the number of elements prioritized for detailed data collection in triage methods, and for developing models to predict materials' impacts.

This work serves as a framework for structuring data to enable streamlined LCA as well as provides guidance for predictive model development. By showing the feasibility of developing effective and efficient taxonomies, the work demonstrates a method to reduce the amount of information required to characterize a product while achieving relatively low uncertainty in the final product impact.

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Table of Contents

List of Figures

List of Tables

1 Introduction

1.1 Motivation

LCA is a methodology designed to assess the environmental impacts of products and services from a systemic perspective. It considers the entire life cycle from materials extraction, manufacturing, transportation, and use through end of life. Due to the structured analytical framework for assessing products that LCA affords, there is a wide array of possible applications for decision-making by consumers, individuals in industry, and governmental organizations. Product design, marketing, and policymaking are a few of the areas discussed in ISO 14040, the governing LCA standard, where LCA can provide useful information (ISO 2006).

This range of applications along with growing environmental awareness has led to an increased demand for results from LCA. Fortune 500 companies now publicly discuss LCA, and trends show increases in the number of LCA publications and downloads (Draucker et al. 2011; Schatsky 2011). It is predicted that a majority of firms will use LCA criteria as part of the purchasing requirements for IT products (Marwah et al. 2011). Furthermore, LCA information is becoming more of a requirement for product sales and marketing as a result of supply chain or governmental protocols, such as Wal-Mart's initiatives and France's *Grenelle* legislation (Schenck 2010).

Despite this growth, performing a LCA remains very resource intensive, and data collection is a challenge for scalability. The process of collecting all the data necessary for conducting a life cycle assessment can be quite onerous and costly. Numerous input values must be collected in order to assess the full environmental impact. Heijungs indicates that this value is around 10,000 points for a "mediocre life cycle inventory (LCI)" (Heijungs 1996). These data are not always readily available, and may require intensive data collection measures or may be outside the control of the party conducting the LCA. For instance, data may be part of the upstream operations within the supply chain, and thus subject to confidentiality concerns (Reap et al. 2008b). Numerous studies have highlighted cost as a problem for LCA, and more specifically data challenges as a main driver of cost (Cooper and Fava 2006; Reap et al. 2008b; Hunt et al. 1998).

Thus, in order to scale environmental assessment, there is a need to find methods to reduce data collection efforts while still being able to achieve usable results. Many streamlining approaches have been proposed, where streamlining within LCA can be considered part of a continuum with "full-scale"

LCA at one extreme (Todd and Curran 1999). Some examples of types of streamlining in attributional LCA include: limiting the scope of the assessment (i.e., limiting or eliminating upstream or downstream stages), using surrogate or secondary data in lieu of primary data, and providing less accurate information for the set of data that does not dominate the results (Hunt et al. 1998; Todd and Curran 1999).

Each of these methods has limitations in its ability to provide information for decision-makers and can introduce uncertainty into the assessment. For instance, although limiting the scope allows for easier data collection, it also requires cutoff of information that limits the potential insights obtained from the result. Many studies have suggested that cutoffs introduce errors and cannot be justified a priori without having collected all of the data (Reap et al. 2008a). Therefore, streamlining methods need to be able to both reduce data collection efforts and have a means of accounting for or incorporating the uncertainty that inevitably results from more limited information.

A plethora of standards have emerged to guide practitioners on how to conduct LCAs and carbon footprint studies (ISO 2006; ISO 2013; BSI 2011; WRI/WBCSD 2011). These provide general guidance on data requirements, boundaries, impact assessment, and reporting. However, they leave room for interpretation by the practitioner and do not adequately address streamlining or appropriate ways to incorporate uncertainty. There is some recognition that challenges exist with collecting data, and that preference is for primary data[1], but secondary data[2] may also be acceptable. Discussion is often vague about how to select secondary data or how to conduct prioritized analysis to determine where secondary data may or may not be appropriate.

More specific standards are being developed within product category groups, called product category rules (PCRs), in order to limit the methodological differences and enable product comparison and consistency. However, even with more specific guidelines, gaps and differences still exist for appropriate use of data and uncertainty. Global harmonization efforts are underway, but standards are not yet ready for mandatory implementation and comparative decision-making (Quantis and Ernst & Young 2010; Subramanian et al. 2012).

[1] Primary data: quantified value originating from a direct measurement or a calculation based on direct measurements of a unit process of the product system at its original source (Quantis and Ernst & Young 2010)
[2] Secondary data: quantified value of an activity or life cycle process obtained from sources other than the direct measurement or calculation from direct measurement (Quantis and Ernst & Young 2010)

This lack of consistency and guidance in the standards relating to streamlining and uncertainty creates an opportunity for methodological development. One option for addressing these concerns is the use of structured data in cases where streamlining is appropriate. An example of structured data would be a hierarchical taxonomy of materials processes. Structured data provides a number of advantages:

1) It is an easy and intuitive way to provide less information in product specification, which will be called under-specification in this work (Olivetti et al. 2013)
2) It creates a structured way to account for uncertainty that incorporates a conservative estimate, and
3) A taxonomy allows inclusion of progressive amounts of information based on what is available to a given user, thus balancing information cost and uncertainty

Many streamlining approaches have attempted to take advantage of data structure (Reis et al. 2011; Meinrenken et al. 2012; Canals, Sim, et al. 2011; Mutel et al. 2009). However, insufficient focus has been placed on the development of the taxonomies, even though this is necessary for performance; better data structures enable lower uncertainty and variation, which in turn lead to higher resolution results. In short, well developed data structures can allow us to make environmental preference decisions with less information.

This thesis explores the use of quantitative methods to develop these hierarchical data structures. It does this by identifying key characteristics for materials classification when multiple environmental impact categories are considered. The structures are then evaluated for how well they account for and reduce uncertainty in the data (effectiveness) and for how little information is required (efficiency). The next section will review literature pertinent to impact estimation when there are data gaps and to the application of classification structures.

1.2 Literature Review

The resource intensity of data collection leads to data gaps when data may be costly to collect. Indeed, data availability and quality was one of the most severe issues that Reap et al. prioritized in their summary review of 15 LCA challenges (Reap et al. 2008a; Reap et al. 2008b). Many streamlining methods have attempted to fill these data gaps and estimate environmental impacts. A summary of approaches will be described in this section as they relate to different types of data for LCA. As the focus of this thesis is more specifically on the formation of taxonomies, more detailed examination of the literature will ensue on how classification and structured data have been explored.

1.2.1 Data Gaps

This section will discuss methods to fill data gaps for four different data types. The first data type pertains to very aggregated environmental impact estimation at the product level. The other three types will be described in parallel and include process data, elementary flow data, and bill of material (BOM) information.

1.2.1.1 Estimating Impact on a Product Level

In lieu of estimating individual data points for a product's components, methods have been developed to estimate the impact of the entire product at once based on databases of similar products. These methods are well suited for early design stages where general insights add more value. Sousa et al. developed artificial neural network based models that used generic product classifications and other product descriptors to create surrogate LCAs. The models used knowable characteristics to generate reasonable predictions of LCI data. The work highlighted the need for additional examination of classification requirements and noted challenges with data availability even in the context of developing these types of models (Sousa et al. 2000; Sousa and Wallace 2006).

1.2.1.2 Quantifying Impact for Data Gaps in Process Data, Elementary Flow Data, and BOM Data

It is more common to attempt to fill data gaps through substitution or estimation of individual process data, elementary flow data, or BOM specification. This section will summarize efforts and challenges with these data types.

1.2.1.2.1 Proxy Data

Use of proxy data is a ubiquitous way to fill data gaps in process data. Accordingly, Cooper and Fava note a heavy use of LCA software and other databases when developing LCAs (Cooper and Fava 2006).

However, this reliance on proxy data introduces a source of uncertainty and subsequent biases in the results that may not be fully understood.

Various methods have been explored to select proxy information where primary data are not available and appropriate secondary database information has not been collected. Methods include direct proxy substitutes, scaling known data to compensate for unknown data, averaging a set of proxy values, or extrapolating from existing data (Canals, Azqpagic, et al. 2011; Wernet et al. 2012). Canals et al. qualitatively highlight the trade-off that exists between the level of effort incorporated and the amount of uncertainty in the result. For example, the first three proxy methods described require less effort, but have a larger amount of uncertainty (Canals, Azqpagic, et al. 2011). The uncertainty and bias is highlighted in another study, which showed that use of surrogate data often leads to a greater than 10% change in the result (Hunt et al. 1998). This level of deviation is often completely unknown at study completion, since the comparison to the "true" result has not been made.

For all of these methods, experts are often required to identify the appropriate criteria for selecting substitutes. Experts provide valuable insights, but can also be expensive and scarce. Furthermore, experts differ in their knowledge, and there has been little study on which are the most appropriate criteria for choosing proxies (Subramanian et al. 2011). Studies that have been done have indicated no general rules for selection of surrogate data (Hunt et al. 1998). Thus, there is a need for additional guidance on the drivers for proxy selection (Canals, Azqpagic, et al. 2011).

1.2.1.2.2 Prediction

Another way of filling data gaps is through the use of predictive methods. Predictive methods use data mining techniques to improve on proxy selection methods and can both be used to estimate process data as well as elementary flow data. One proposed method used neural network models with molecular structure properties to predict the environmental impacts of chemicals. All chemicals' impacts can be estimated with the model, or alternatively, a screening process can be used to identify the most impactful chemicals for which process data would be substituted in lieu of the predicted values (Wernet et al. 2012; Wernet et al. 2008). This method showed benefits in chemical inventory development, but was not applied to other materials. Furthermore, one drawback of neural network models is that they obscure relationships between variables and impacts, and can make it difficult to determine the true drivers of the impact.

Similarly, other prediction methods for process data use fundamental materials properties to understand their impacts. This has been applied in quantitative structure activity relationship (QSAR) models, which use multivariate methods to predict properties of chemicals, such as chemical toxicity, based on specific material properties (Oberg 2004). More complicated models have been used in computational materials science to predict multi-attribute materials properties based on ab initio modeling with first-principles, such as quantum mechanics or thermodynamics. One application of this type of model has been to reduce laboratory experimentation efforts and identify the best candidates for Li battery materials (Ceder 2010; Hautier et al. 2011). Although this work has not been performed in the LCA domain, similar concepts could potentially be applied. The work described in this thesis however seeks to identify more "knowable", emergent properties, but could potentially be expanded in the future.

A final process prediction method mapped BOM information to environmental impacts and used medoids (i.e., the most representative points) of the groups to predict impact (Marwah et al. 2011; Sundaravaradan, Marwah, et al. 2011). This does simplify the prediction, but does not capture the uncertainty present in the groups.

Elementary flow data often comprises thousands of substances, leading to burdensome data collection. In lieu of predicting impacts from a process perspective, other studies have sought to reduce data collection by identifying key elementary flows. Lasvaux et al. used regression to select the key elementary flows for abiotic resources depletion potential, limiting analysis to just nine flows (Lasvaux et al. 2010). Another method used cumulative energy demand (CED) as a means to predict other impacts through regression models, since CED requires collection of fewer elementary flows than other impacts (Huijbregts et al. 2006). Although this reduced the effort, there is still a lot of unexplained variation in some of the models, and challenges remain in just collecting the data required for CED.

1.2.1.2.3 BOM Specification

Beyond the simplification methods described above, sometimes simply characterizing the BOM of a product can be challenging. Without the BOM information, proxy and prediction methods are difficult to apply. The collection of BOM information is particularly challenging for highly outsourced and complicated products, where collecting upstream information through the supply chain can be resource intensive. One way of reducing the effort is by grouping BOM components to require specification of fewer parts. This has been shown to be feasible through clustering methods (Marwah et al. 2011;

Sundaravaradan, Marwah, et al. 2011). Alternatively, the same studies have used a "reverse engineering" type method with data mining techniques to predict BOMs through tree discovery given a final impact (Marwah et al. 2011; Sundaravaradan, Patnaik, et al. 2011; Sundaravaradan, Marwah, et al. 2011).

Other proposed methods required less information to characterize the BOM, and then subsequently predicted impacts based on abstracted materials categories. One of these is streamlining through product-attribute-to-impact-algorithms (PAIA), where materials were specified in groups (e.g., metals) and sampled to predict their impacts (Reis et al. 2011). Another method called fast carbon footprinting used similar data structures to streamline prediction of product carbon footprints (Meinrenken et al. 2012). These methods are reliant on the underlying data structure, and limited study has been conducted to identify the best way to construct this structure. Furthermore, efforts have been limited only to the carbon footprint and have not yet been extended to other environmental impacts.

1.2.1.2.3.1 Under-specification as a Method

The concept of using the structured data in conjunction with uncertainty as a means of streamlining has been more formally described by Olivetti et al. as probabilistic under-specification. This process involved two parts (Olivetti et al. 2013):

1) Under-specification – A product component is characterized by available information about materials characteristics rather than by specific process based data, then is fit into a hierarchical data structure, and Monte Carlo simulation is used to sample all the possible proxy values that correspond with the group identified in the hierarchical data structure.
2) Probabilistic triage – The set of interest (SOI) is identified to indicate where more targeted and detailed data collection should be performed for better resolution of the results.

An example of a data structure for under-specification is shown in Figure 1-1. Here, the metals are described at five different levels of specificity based on the amount of information available to the user. As you progress to higher levels of specificity, the cost of providing the information increases. However, there is a trade-off in that the uncertainty will ideally decrease. This method, unlike other streamlining methods, provides a way to estimate uncertainty at different levels of specificity (Olivetti et al. 2013).

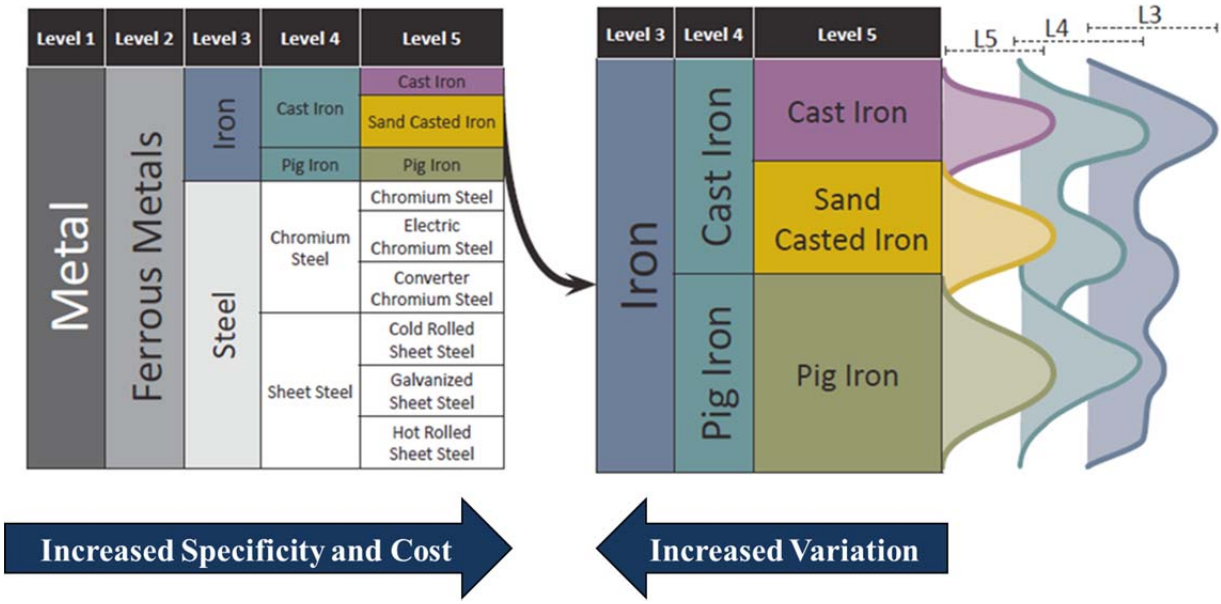

Figure 1-1. Example of under-specification structure and the abstraction of the uncertainty from sampling within the groups. Adapted from (Olivetti et al. 2013).

The work by Olivetti et al. demonstrated benefits of reduced data collection from under-specification and especially the use of probabilistic triage to identify the SOI. However, as mentioned, it did not focus on the best way to group materials to balance this trade-off between cost and uncertainty. Hierarchical structures were based on qualitative evaluation of existing surrogate data structures rather than quantitative mapping or data mining methods. Another study that applied the under-specification method to food related processes emphasized the need for increased focus on development of data structures. Lee found that poor data structures reduced accuracy in streamlining (Lee 2013). Another limitation of the work by Olivetti et al. was that the examination of structures was based solely on the CED rather than the wider range of impacts relevant for product evaluation. Thus, there are opportunities to build on this assessment to support application of under-specification and streamlining methods more broadly.

1.2.2 Classification Structures

As the development of classification structures is relevant to this work, the literature was also evaluated to identify other ways that classification structures are currently used. The scope of this analysis focused predominantly on applications within the LCA domain, but other fields have used hierarchical structures as well.

1.2.2.1 Product Classification

Multiple methods were used to group products, often for use in other predictive algorithms such as neural network models. Park and Seo identified multiple grouping methods based on clustering of products by hierarchical analysis of product attributes, on impacts of various life cycle phases, on top indicator classes, and on functional properties of the products (Park and Seo 2003). Sousa et al. used hierarchical clustering and classification schemes to group products based on product attributes (Sousa and Wallace 2006). Soriano clustered based on the percentage of impacts from different life cycle phases (Soriano 2004). Lastly, Kaebernick and Soriano clustered on both product characteristics and environmental factors (Kaebernick and Soriano 2000). Many of these studies grouped products based on the relative impacts in the use phase and in materials production. Other factors were also identified such as functional application and fiber content. Hierarchical clustering was a common method used to identify the groupings, although the specific variables used in the algorithm differed between studies.

1.2.2.2 Elementary Flow Classification

In addition to classification of products, elementary flows can also be grouped for similarity. One study examined the grouping of elementary flows using k-means clustering analysis. The goal of this work was to create flow archetypes to be able to more accurately characterize uncertainty factors for these flows (Muller et al. 2012). This provides another example of clustering as a means of grouping items for LCA streamlining.

1.2.2.3 Material Classification

Lastly, classification of materials is considered. Some examples of this have been described previously in Sections 1.2.1.2.3 and 1.2.1.2.3.1. Other studies have used analogous philosophies of grouping similar materials to be able to characterize less information in analyses. One example was a study which explored greenhouse gas assessments at a portfolio level for soups. Ingredients were organized into typologies to streamline the assessment. The study identified the need to better assess groupings of the ingredients (Canals, Sim, et al. 2011). Another study by Mutel categorized fruits and vegetables according to qualitative groupings. It found that there was as much variation within groups as between groups, and thus, more exploration was needed to inform material classification (Mutel et al. 2009).

Clustering has also been applied to group materials. Johnson et al. explored the use of clustering based on technical and aesthetic properties from the Cambridge Engineering Selector (CES) database. These properties were used to create groups that would aid in materials selection for designers (Johnson et al.

2002). Other work by Ashby has focused on relating technical properties to environmental impacts by visual groupings on property plots (Ashby 2005). These plots are used for a design focus, and are easiest to interpret with only two dimensions.

Lastly, clustering of materials has been specifically applied to group materials based on environmental impacts. Sun et al. grouped metals classes by their eco-indicator single score both graphically for visual segregation and through hierarchical clustering methods. Using these methods, they identified appropriate groups for the materials and found reductions in coefficient of variation (COV) (Sun et al. 2003). Although this work seeks to address the problem of quantitatively creating classification structures, it suffers from a few limitations. One, it does not always seek to create groups based on knowable characteristics, but more based on the clusters created (e.g., for non-ferrous metals categories). Secondly, it uses a weighted score that limits the ability to understand how groupings relate to individual environmental impacts.

1.3 Gap Analysis

Creating classification structures with materials has been identified as a promising method for streamlining by many different studies. However, given the impact of the underlying structure on the ability to streamline effectively, there is an overall consensus that more research is necessary on how to best structure material groups to suit streamlining needs. The work in this thesis seeks to address this gap by applying quantitative methods to explore how hierarchical classification structures might be formed. It builds on previous use of clustering analysis to understand the creation of taxonomies. It further expands previous exploration of structures from a single impact to a multi-attribute analysis of environmental profiles.

1.4 Central Question

This research proposes a meta-analysis of inventory process data to identify key classifiers that are relevant to the creation of hierarchical classification structures and predictive models for filling LCA data gaps. This research examines how quantitative data mining methods can be used to identify and evaluate these classifiers. This is applied through the use of exploratory analysis methods, expert judgment, and modeling based methods.

These analyses explore the question of whether or not quantitative methods can be used to inform the development of effective and efficient classification structures. Effectiveness relates to the reduction of uncertainty across the data structure as well as accuracy of the result, addressing the following three questions:

1) How close is the "predicted" impact for a given material to its "true" impact, or in other words, what is the percent error from the individual database entry?
2) For what percentage of materials does the percent error decrease when more information is provided in the taxonomy?
3) What is the uncertainty of the proposed groups in the taxonomy, and how does it change as more information is provided?

Efficiency pertains to the amount of information and the value that it provides, related to these questions:

1) What is the "cost" of information required to identify where a material falls in the classification structure?
2) Are the groups created in a given level of the taxonomy distinct from other groups in that level, thereby demonstrating the value of the additional information and the ability to distinguish materials?

Specific metrics to evaluate the proposed taxonomies for each of these questions will be discussed in the methodology section.

Beyond this evaluation of potential taxonomies, we further want to analyze:

- Which classifiers are the best for characterizing a material's environmental profile, and does this change based on the material type under consideration?

- How is the development of the classification structure observed to be affected by the consideration of multiple environmental impacts simultaneously rather than a single one?
- What challenges exist in creating classification structures that may limit the applicability of this type of methodology?

These additional questions will be addressed within the discussion section.

1.5 Thesis Outline

In this thesis, we propose a methodology to create effective and efficient materials taxonomies.

Chapter 2 describes the methodology developed to conduct exploratory analysis, identify and evaluate potential classifiers, create and assess materials taxonomies, and apply the structures to case studies.

Chapter 3 provides examples of the taxonomy creation methodology as applied to three materials datasets: metals, polymers, and precious metals.

Chapter 4 then shows a case study using these taxonomies in a streamlined application via under-specification. This section also presents examples of using the classifiers from Chapter 3 in predictive models.

Chapter 5 discusses the results found as well as the successes and limitations of the methodology.

Chapter 6 summarizes conclusions and is followed by a list of relevant literature and appendices.

2 Methodology

The goal of the analysis was to produce an effective and efficient taxonomy of materials to be used in streamlined assessment. The analysis considered multiple environmental impacts simultaneously to create hierarchical structures that allow under-specification to be used effectively for a wider range of applications. This work identified the key characteristics, or classifiers, for improved materials classification when multiple impact categories were considered. It further explored how data mining approaches can be used to determine these classifiers in order to both inform taxonomy formation and predict performance.

To achieve this, a dataset including materials and their potential classifiers was generated. Classifiers in this context will be defined as characteristics that allow the identification of a member of a group. Using this dataset, the initial analysis consisted of two main parts:

1) Exploratory analysis of the data along with expert judgment to identify possible classifiers related to underlying patterns in the data, and
2) Evaluation of those classifiers for their potential for uncertainty reduction and predictive abilities

The results were translated into a taxonomy or hierarchical structure, which was also statistically evaluated for performance. This process may be iterated multiple times to generate the appropriate list of classifiers and create taxonomies.

The next part of the analysis involved using the resulting taxonomy or taxonomies to evaluate a case study. The bill of materials was under-specified for the two examples using the hierarchical structures created, and the uncertainty of the results was considered. Better resolution in the results allows for improved product differentiation. The identified classifiers were also used to create predictive models for the environmental impacts of both metals and precious metals. A summary of the methodology is shown in Figure 2-1 and described in more depth in the following text.

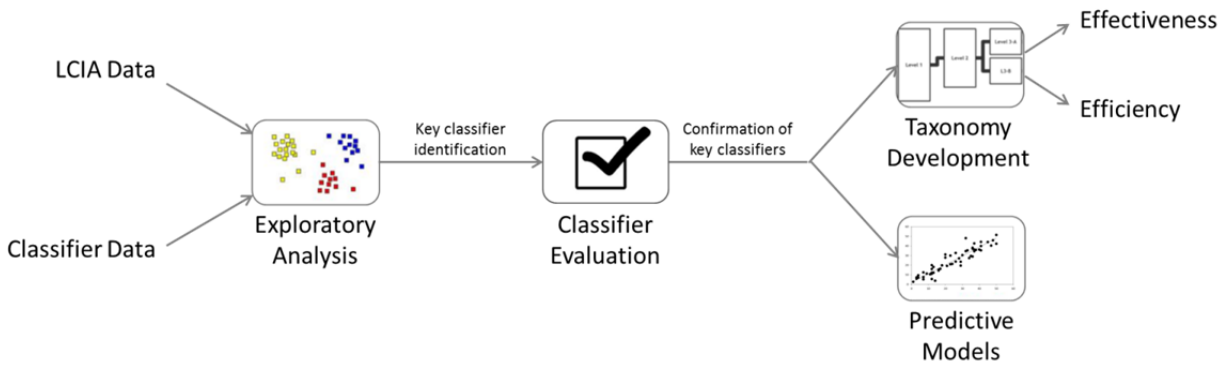

Figure 2-1. Summary of the methodology for the development of hierarchical taxonomies and predictive models. Although, not illustrated as such for ease of interpretation, this process is iterative and can include progressive improvements.

2.1 Dataset Formation

2.1.1 General Data

Creation of taxonomies requires evaluation of a wide range of data to best identify patterns and trends. To achieve this, data were derived from a combination of publicly available LCI datasets. These included European Aluminum Association (EAA), European Copper Institute (ECI), Ecoinvent 2.2, European Reference Life Cycle Database (ELCD), Eurofer, GaBi 5 database from PE International, International Copper Association (ICA), Industry Data 2.0, LCA Food DK, PlasticsEurope, United States Life Cycle Inventory (USLCI), and World Steel (PE International AG 2011; EAA 2008; EMPA 2010; JRC of the EC 2008; Eurofer; NREL 2012; World Steel Association 2011; PlasticsEurope 2009). Boundary conditions are set within the individual datasets, and so differ amongst them. The goal was to have a broader and more representative dataset, so all were used despite the differences in boundaries, allocation, etc. All materials were evaluated based on a 1kg functional unit. If no conversion to weight existed, the material was excluded from the study.

A number of the databases use similar underlying LCI data and data sources for calculations. Efforts were made to remove duplicates except where they seemed to differ in impacts inconsistently with data derived from the same source. For instance, many of the polymers databases used similar underlying data, but the evaluated impacts did not always track consistently. Where it could not be determined how the data may have been adapted, the data were included in the dataset.

Although these databases did make up a reasonable amount of data for analysis, a few caveats should be made. Ideally, data would have been randomly sampled from the entire population of materials based on their prevalence of use. This was not possible to do, since data were not available for all materials, processing conditions, production locations, etc. Thus, the analysis will not be fully representative of all materials and some may be oversampled within the dataset. This may have led to error and over-fitting in certain cases. Attempts were made to mitigate these effects through validation samples, but some effect was unavoidable. Furthermore, the non-ideal sampling meant that some possible classifiers and characteristics were not possible to evaluate due to a lack of data. Thus, the representativeness of the structure as new data are collected should be evaluated for continued applicability. Lastly, as mentioned, the boundary conditions differed between datasets. This manifested in some residual error in evaluating classifiers, mostly related to the source of the data. Again, this

effect was unavoidable, as our objective was to work with a larger dataset, but some methods to diminish data source effects will be discussed.

2.1.2 Environmental Impact Selection

To apply the method in this work to streamlined footprint calculations, each database entry was evaluated at the midpoint level using TRACI 2.0. The life cycle impact assessment (LCIA) was applied within either SimaPro and GaBi depending on which contained the database. TRACI 2.0 was selected to provide a range of midpoints to assess, and because of its relevance to North America, where the research was conducted (Bare 2011). Error associated with the impact categories was not propagated through, and so the impacts evaluated are based on the magnitudes of the characterization factors applied to each elementary flow using TRACI 2.0.

No official normalization or weighting was applied to the midpoints for analysis. However, for evaluation of the environmental profile of the materials, an inherent weighting assumption was required for certain data mining methods. In these cases, all midpoints were determined to be equal. This was a value judgment and could be altered to apply weighting based on the needs of the user. Different structures may be created depending on the desired weighting. Unfortunately, all impacts from TRACI 2.0 could not be included due to challenges with data source error, which will be described in more detail in Section 3.1.1. Analysis here focused on a subset including:

1) Acidification (mol H^+ equivalent)
2) Global warming potential (kg CO_2 equivalent)
3) Human health non carcinogenic (CTUh) , and
4) Smog formation (kg O_3 equivalent)

Theoretically, analysis is possible at the life cycle inventory level to determine similarity in materials and datasets. If this methodology were to be applied at the inventory level rather than the impact level, the analysis would become highly multi-dimensional. This wide range of variables could create sparse data spaces that would make interpretation and analysis more difficult (Tan et al. 2005). Thus, dimensionality reduction may be desired in these cases. This can be achieved through application of principal component analysis (PCA). Applying PCA to the dataset could identify a few key principal components that account for most of the data variation, and those could be used for further analysis. Alternatively, distance metrics that account for correlation could be used with the exploratory data mining techniques that will be described in this section. In this thesis, dimensionality reduction was not

employed due to the smaller set of impacts evaluated, but these notes are included here for completeness in how this methodology could be applied in the future.

2.1.3 Classifier Data

The word classifiers will be used throughout the following sections. Classifiers may refer to properties or attributes of each of the materials. They will be used to identify ways that the materials may be grouped to create taxonomies. Three main types of classifiers were considered in the analysis:

1) Characteristics of individual process datasets (e.g., recycled content, database source)
2) Qualitative categorization of materials (e.g., function, polymerization method)
3) Materials properties (e.g., price, tensile strength, density)

The analysis strives to identify key classifiers that can characterize the uncertainty and are "knowable". Focus has been placed on manufacturers of products rather than end users, and the classifiers are evaluated from this perspective. Thus, price is the price of the materials rather than the price of an end product. This reduces some uncertainty in classifier values due to value added factors from manufacturers, such as intellectual property. We also did not focus on end product attributes, but rather material attributes.

The classifiers to be collected were identified in the exploratory step of the methodology. They were collected from a variety of sources including the documentation for the LCI databases, materials literature, and property data included in the CES database (Granta Material Intelligence 2012). Both continuous (e.g., price) and categorical (e.g., function) classifiers were evaluated. However, in the end, all needed to be translated to categorical groups to be able to create a taxonomy. In the evaluation stage, some data mining techniques applied could accommodate both types of classifiers, whereas for others, classifiers had to be converted to one type or the other.

2.2 Exploratory Analysis and Classifier Identification

The first step in the methodology was to conduct exploratory analysis of the dataset. Exploratory analysis here includes both data visualization to better understand patterns in the data as well as application of unsupervised data mining methods. Unsupervised data mining methods seek to identify underlying patterns in the data, but have no target variable that they are seeking to explore for predictive capabilities. These types of methods do not require assumptions a priori about which variables (here classifiers) should be used; they allow an opportunity to examine the data and identify which variables might be useful in the analysis. As there is a multitude of ways that materials may be grouped, these types of unsupervised methods provide a very useful starting point for the analysis. Two methods will be described in more detail in this section: clustering and principal component analysis. An additional discussion of outliers and influential points will follow.

2.2.1 Data Visualization

Data visualization was first used to identify patterns in the data and to recognize parameters requiring transformation. This analysis was performed in JMP and R to analyze both scatterplots for continuous variables and boxplots for categorical variables. Visualization offered insights into influential points within the data. Furthermore, ranking of the data by impact supplemented this understanding. These analyses were useful, but do not substitute for methods that will be described (e.g., clustering), since clustering considers all impacts simultaneously, whereas it may be difficult to assess multi-attribute criteria by inspection alone.

2.2.2 Principal Component Analysis

Principal component analysis (PCA) was also examined as an exploratory method for identifying important patterns in the data. PCA has previously been used within LCA (Pietrzykowski 2009; Basson and Petrie 2007). PCA is a useful method for reducing dimensionality by identifying a set of orthogonal principal components (PCs), which capture the variation of the original dataset (Joliffe 2002). Additionally, PCA can be used to identify potential outliers, influential data points, and can be used to suppress noise by re-computing the original data space by disregarding PCs showing large noise components.

In this analysis, PCA was conducted in R using the midpoints, which were standardized by the mean and standard deviation. The biplot of the first two PCs was examined to identify potential outliers and influential points. These were used to identify possible classifiers, as appropriate classifiers need to

account for factors that differentiate these points. PCA was also useful to show how materials were grouped within the data space (e.g., those that varied more in global warming potential versus non carcinogenicity).

2.2.3 Clustering

Clustering analysis is one of the main unsupervised methods which group data items based on their similarity. Ideally it also identifies groups that are distinct from one another. Clustering has been applied in many fields such as biology, market segmentation, and medicine (Izenman 2008). Clustering has been used more specifically within LCA to identify data gaps, fill in missing information, enable more rapid assessment of large BOMs, and enable product or material classification (Marwah et al. 2011; Sundaravaradan, Marwah, et al. 2011; Pietrzykowski 2009; Sun et al. 2003; Kaebernick and Soriano 2000; Soriano 2004; Sousa and Wallace 2006). In this work, clustering was the most important method used in the exploratory analysis.

2.2.3.1 Randomness Check

Cluster analysis will identify groups within data whether or not they are present. Thus, it was first useful to check whether the data were random or not, and therefore whether clusters would provide any valuable information. Randomness was evaluated using the Hopkins statistic, a statistical clustering tendency metric. This metric compared nearest neighbor distances to original data points for both randomly generated points across the n-dimensional data space and for randomly samples points from the dataset itself. Multiple trials were run, and the value was used to assess the degree of clustering tendency in the space; the closer the Hopkins statistic was to zero, the higher were the clustering tendency of the data (Tan et al. 2005). Hopkins statistic, *H*, is defined as:

$$H = \frac{\sum_{i=1}^{p} w_i}{\sum_{i=1}^{p} u_i + \sum_{i=1}^{p} w_i} \qquad \text{(Eq 1)}$$

where w_i is the distance to the nearest neighbor for the points sampled from the original dataset, u_i is the distance to the nearest neighbor for points randomly generated in the data space, and p is the number of points evaluated per trial.

2.2.3.2 Clustering Algorithms

Once it was ascertained that the data were not random, clustering was conducted. There are many clustering algorithms available to evaluate data. Some of the more popular methods include partitioning and hierarchical methods. Partitioning algorithms, such as k-means clustering, divide data

into distinct groups. Hierarchical algorithms create a tree structure of the data, and thus divide data into nested groups.

For this analysis, focus was placed on the use of hierarchical algorithms for a few reasons. First, the end goal of the analysis was to be able to create a hierarchical classification structure. Second, the number of clusters was unknown a priori, which is a requirement for partitioning methods, such as k-means. Lastly, k-means clustering was explored across a range of different numbers of clusters, and the best results based on evaluation metrics incorporated too many clusters to be useful in the exploratory stage. Although it is often useful to explore multiple clustering methods to understand data, here the goal was not to identify "true" clusters in the data, but rather glean possible classifiers for future evaluation. Thus, a single method was deemed sufficient for the analysis.

Hierarchical methods vary in the distance metrics used to assign groups. As the goal of this assessment is to reduce uncertainty in the majority of individual groups across/along the taxonomy, the Ward method was chosen. This method minimized the sum of squares at a given step. The values used to do the clustering analysis were the environmental midpoints evaluated by TRACI 2.0. Due to differing measurement scales and levels of uncertainty between the set of midpoints, the impacts were standardized by the mean and standard deviation prior to incorporation. This maintained the prior assumption of equality between the midpoints rather than placing more weighting on midpoints with higher orders of magnitude. Clustering was performed within the JMP software.

2.2.3.3 Cluster Evaluation

As hierarchical clustering produces a tree of data items, the tree branching can be ended, or cut, at multiple points to evaluate clusters. The best number of clusters was selected by examining the knee in the joining distance scree plot. This plot looks at the distance to join the next group in an agglomerative hierarchical algorithm. The knee identifies the point where little more can be gained by adding more clusters and the distances level off. Additionally, cluster evaluation was also considered at a cut where the largest distance gains (cluster differences) had been realized. The taxonomies created in this work have multiple levels of information, which add specificity with progression through the levels. The cut with fewer clusters can be used to identify initial data classifiers and earlier levels in the taxonomy, whereas the cut in the knee can show potential future groups for later levels of the taxonomy.

Clustering shows how groups differ by their environmental profile and distinguishes materials that may be significant in certain impacts. The analysis only identifies exploratory groupings within the data, so it

is up to the user to identify key characteristics describing each group and differentiating it via its impacts. Some validation methods do exist to compare metrics to the clusters, however these can be difficult to interpret and may be inconsistent to apply (Tan et al. 2005). Therefore, expert judgment, which will be described in more detail, is useful to examine unifying themes within clusters to indicate possible materials classifiers that may not have otherwise been considered.

Lastly, outliers were considered. Analysis showed that the clustering methods were very successful at identifying the outliers or influential points within the data when analyzing the untransformed data. If the data were log transformed, the effect of the outliers was lessened. Thus, data may be clustered twice: once to identify influential data points and a second time to identify typical groupings within the data. The main focus in this work was placed on clustering untransformed data to make sure that outliers were accounted for, and because streamlined application of the structure through under-specification is conducted in the untransformed space.

2.2.4 Outlier and Influential Point Identification

Outliers and influential points can have a significant effect on the end variation of the data, so they needed to be considered upfront. Here we will refer to outliers as points that significantly deviate from the rest of the data and influential points as higher impact points within the tail of a skewed distribution. While outliers may be excluded from the dataset or further examined for accuracy of the data, influential points are real parts of the data that must be accommodated in the classification. PCA, clustering, and boxplots helped to identify both types of points for characterization. The Mahalanobis distance test provided additional confirmation of outliers by evaluating multivariate properties of the data to determine those points which had higher distances.

2.2.5 Expert Judgment

Exploratory methods provide insights into the patterns in the data, but do not provide a decision variable to use for prediction or classification. Furthermore, the groupings created from clustering, while useful from a data perspective, were not necessarily intuitive, and so may make it difficult for a user to identify an appropriate group for a prospective material. Thus, the previous methods must be combined with expert judgment in order to actually create the desired taxonomies. Experts in life cycle assessment, materials engineering, and chemistry were consulted to help identify the key characteristics, or classifiers, that might be able to describe a given cluster or distinguish clusters from one another. Furthermore, they were asked about ways to group materials that might make intuitive

sense for the materials categories explored. As expert judgment is subjective, consultation with a broader range of experts could provide additional insights into the key characteristics of the data.

2.2.6 Iteration

Since intuitive groups identified through expert judgment may differ from those created through direct clustering of the data, strictly using the hierarchical nature of the first clustering results was insufficient. After a first level of information was determined, the process described above was iterated on each of the groups in the first level in a tiered type approach. This can be repeated for any number of levels. Discussion in Section 3.1.5 will explain that two iterations were used in this thesis to produce a four level taxonomy, where the first level is the material type, the fourth level is the database entry, and the second and third levels were a result of this analysis. The exploratory part of the analysis produced a list of influential materials and possible classifiers identified through expert evaluation of the data mining results, which will be further evaluated in subsequent sections.

2.3 Classifier Evaluation

Materials may be grouped in many ways to identify similarity, and it is difficult to know which groupings are most related to the environmental impacts (Canals, Azqpagic, et al. 2011). The exploratory analysis generated a list of possible classifiers to consider for these groupings. Additionally, to further support expert judgment described above, it is beneficial to evaluate the dataset to identify which of the possible classifiers are best suited to taxonomy creation and/or predictive purposes. In this study, the classifiers were examined to identify which reduced the uncertainty the most (effectiveness) while requiring little information input (efficiency). Multiple measures of uncertainty exist, and so a few methods were explored to afford a more complete sense of the data and the trends within the dataset. A single method would provide a limited perspective of the data, but using many methods offers a more holistic picture. One drawback to this approach is that multiple measures can indicate different outcomes and preferred classifiers.

Both continuous and categorical classifiers were considered in the evaluation. Continuous classifiers were evaluated for their contribution to the uncertainty. The most relevant in terms of uncertainty contribution were translated into categorical classifiers to enable the creation of hierarchical data structures. The classifiers were evaluated based on five methods, which are summarized in Table 2-1, and described in the subsequent sections. In each method, the top performing classifiers were identified. The results of explorations across all methods were aggregated to analyze the frequency of contribution for a given classifier. Those that were most frequently important were later used to create possible taxonomies for evaluation.

Table 2-1. Summary of metrics used to evaluate classifiers

Uncertainty Based Methods	Modeling Based Methods
1. Comparison to rotated scores from PCA	3. Linear regression
2. SSW/SST	4. Logistic regression
	5. Regression trees

Data were log transformed for this portion of the analysis, as it is important to underlying assumptions in several of the methods. Furthermore, transformation can provide more useful information about patterns in the data, particularly related to predictive measures, since the transformed data are not as heavily influenced by the outliers present in the data.

In evaluating classifiers, ideally all of the above methods would consider the environmental profile of each material. However, this was infeasible, as some methods required a single dependent variable and could not handle the multivariate nature of the data. Thus, for some methods (specifically, methods 3 and 5), the environmental impacts were combined into a single dependent variable for analysis. To create the single dependent variable, each environmental impact was standardized by the mean and standard deviation, and all were added together. This did obscure some of the desired information, but allowed for the use of more methods to understand relationships.

2.3.1 Uncertainty Based Methods

Multiple uncertainty based methods were examined to understand how the classifiers accounted for the uncertainty and variation in the data. These each provided slightly different information about the nature of the variation.

2.3.1.1 Principal Component Analysis

As described in Section 2.2.2, principal component analysis identifies orthogonal principal components accounting for the variation in the dataset. As this method sought to find classifiers that accounted for the main sources of variation and reduce the uncertainty within the dataset, examining how the classifiers compared to rotated scores from PCA was useful. The first few principal components (PCs) generally account for a large portion of the variation in the analysis. Thus, the correlation of potential continuous classifiers with these PCs was explored to see which classifiers contributed the most to each portion of the uncertainty. For categorical classifiers, graphical examination of the distinction between groups was observed. Distinction here is described as the ability to visually differentiate the distributions of the PC values across categories for a given classifier.

2.3.1.2 Decomposition of Variance – SSW/SST

One way to examine the variation in the dataset is to decompose the variance into its constituent parts. Categorical classifiers break the data into groups, and both the variation within groups and between groups can be evaluated. The within sum of squares (SSW) is calculated using Equation 2:

$$SSW = \sum\sum\left(y_{ij} - \bar{y}_j\right)^2 \qquad \text{(Eq 2)}$$

where y_{ij} is the value of one environmental midpoint for a given data point and $\bar{y}_j$ is the mean of the environmental midpoint for the group of which that data point is a part. If the sum of squares within is

added to the between sum of squares (SSB), this is equivalent to the total sum of squares (SST), which is shown in Equation 3:

$$SST = \sum\sum\left(y_{ij} - \bar{\bar{y}}\right)^2 \quad \text{(Eq 3)}$$

where $\bar{\bar{y}}$ is the grand mean value of the environmental midpoint for the entire dataset. Thus, if the SSW is normalized by the SST, this will indicate the residual error present in the groups created by a categorical classifier. This also provides an easy to interpret value representing the percentage of the total error that remains after the "treatment". As the SSW and SSB are additive, reduced error within groups also translates to more distinction between groups.

These SSW and SST metrics are typically used within analysis of variance (ANOVA) problems. ANOVA has been applied in many fields, including within agriculture to identify the highest yielding wheat variety (Albright et al. 2004). It can be used in both experimental and observational studies. The first is preferred, but unfortunately we had only observational results, and so could not fully control the sampling of the values amongst the groups.

This metric can be calculated across environmental midpoints and summed to provide a single percent of the total variation remaining after grouping using a categorical classifier as in Equation 4. As continuous classifiers must be translated to categorical classifiers for taxonomy creation, this metric is one option for selecting threshold values for translating continuous classifiers into categorical ones. Furthermore, the use of squared distances emphasizes the impact of outliers, and so optimization with this metric will reduce the influence of outliers.

$$\frac{SSW}{SST} = \frac{\sum\sum\left(y_{ij} - \bar{y}_j\right)^2}{\sum\sum\left(y_{ij} - \bar{\bar{y}}\right)^2} \quad \text{(Eq 4)}$$

2.3.2 Modeling Based Methods

In addition to considering the uncertainty and variation, multiple prediction models were applied to evaluate classifiers. These methods allowed for supervised assessment of the classifiers and, in each case, data were divided into training and validation portions to enable selection of the best models. Each method relied on different assumptions that again provided unique information about the dataset.

2.3.2.1 Linear Regression of a Continuous Variable

Regressions methods provide a simple and easily interpreted method of predicting the performance of a continuous response variable. Due to their ease of use, they have been applied in many applications, including in LCA. One study used cumulative energy demand (CED) as an independent variable to predict a range of environmental impacts for materials production, energy production, transportation, and waste treatment processes in linear least squares regression (Huijbregts et al. 2006). Further work has built on the analysis by Huijbregts et al., and other studies have also used regression as a means of predicting life cycle bill of activity information or life cycle impacts based on product attributes (Padey et al. 2012; Park and Seo 2003; Murphy et al. 2003; Hanes et al. 2013; Reis et al. 2012). Similar analysis has been conducted using parameterization type models (Cooper et al. 2012).

In this thesis, regression was used in a similar fashion to predict life cycle impacts based on material attributes and properties. Analysis was performed in JMP, and ordinary least squares regression was used with continuous classifiers and dummy variables created from categorical classifiers as the explanatory variables. The dependent variable was the combined standardized environmental midpoints, where the standardization method was the same as for clustering. 20% of the data were randomly selected to comprise the validation dataset. A stepwise procedure was used to identify a few possible regression models. Determination for inclusion of classifiers in the models considered the p-values of each parameter (or partial F-test p-values for sets of parameters) and variance inflation factors (VIFs) for the expected multicollinearity of the parameters, and examined the coefficients for reasonableness.

These models were then evaluated on a number of parameters. First, the R^2 value was considered to determine how well the model accounted for the variation in the environmental impact of the training data. The adjusted R^2 value was considered in model selection as well to avoid overfitting of the data. The residuals were examined for any patterns and for normality to ensure that the assumptions were met and that the model was an accurate representation of the data. Lastly, error metrics were used to identify the best model using the validation data. Two metrics were considered; first the mean absolute error (MAE), as shown in Equation 5:

$$MAE = \frac{1}{n}\sum|y_i - \hat{y}_i| \qquad \text{(Eq 5)}$$

where $\hat{y}_i$ is the predicted value for the dependent variable, y_i is the actual value, and n is the number of samples. The second metric was the root mean square error (RMSE), as shown in Equation 6:

$$RMSE = \sqrt{\frac{\sum(y_i - \hat{y}_i)^2}{n}} \quad \text{(Eq 6)}$$

2.3.2.2 Logistic Regression

Logistic regression uses the inverse of the linear regression; the environmental impacts are the explanatory variables and the proposed classifier is the dependent variable. For this analysis, all classifiers must be translated into categorical classifiers. The method estimates the probability of belonging to a group based on minimizing the negative log-likelihood (JMP 2012). Multiple classification methods exist, and logistic regression was selected because it does not assume multivariate normality. Thus, it is more robust to deviations in the dataset. This work used nominal logistic regression as applied in JMP.

As with the linear regression analysis, 20% of the data were randomly sampled to be reserved as a validation dataset. Sampling was not stratified due to the desire to compare multiple classification options. This may have resulted in some categories being over or under-sampled in the evaluation, but provided more consistency in the analysis. Each environmental midpoint was used as a separate explanatory variable to be able to account for the environmental profile of the materials. Models were analyzed based on their accuracy in classification rates. The baseline value was the percent accuracy assuming all items belonged to the largest group. The improvement metric showed how well a given model improved on the baseline as in Equation 7:

$$\%\ Improvement = \frac{(\%\ accuracy - baseline)}{(1 - baseline)} \quad \text{(Eq 7)}$$

The results from the validation data analysis were used to identify the best classifiers from this method.

2.3.2.3 Regression Trees

Classification and regression trees (CART) were the final prediction method used in this analysis. Classification trees predict categorical values, and regression trees predict continuous variables. Here, regression trees were used to predict environmental impacts, where the dependent variable was the same as for linear regression. This algorithm is based on recursive partitioning, where a given group or node on the tree is broken into two parts in a step by step procedure. The data space is broken into

uniform non-overlapping sections (Izenman 2008). The result is a tree that provides decision rules for determining which group items fall in. For regression trees, the predicted value is the average value within a leaf of the tree. Methods for growing and pruning the tree to determine the right tree size must be determined, since a large tree may tend to overfit the data, whereas a small tree may not capture important patterns in the data (Hastie et al. 2009).

Classification and regression trees have been used in many applications, such as biomedical research, medical diagnosis, botany classification, marketing, and decision theory (Izenman 2008; Saldivar-Sali 2010). Regression trees provide a number of benefits, such as usefulness in exploration without prior models, interpretability, and ability to handle large datasets (JMP 2012). Furthermore, they can accommodate both continuous and categorical classifiers simultaneously, they do not require distributional assumptions and are non-parametric in nature, they can identify possible threshold values to translate continuous classifiers into categorical ones, and they create a tree structure, which is the goal of this analysis (Saldivar-Sali 2010). However, one consideration was that the splits may be sensitive to small changes in the data and what has been sampled. For this reason, cross-validation was used to assess these models instead of simply a validation dataset.

The regression tree analysis was performed using the partition method in JMP. This grew a tree based on the LogWorth ($-\log_{10}$(p-value)) splitting method, where the p-value accounted for multiple options for splitting. The tree growth stopped when the R^2 was better than would be achieved with the subsequent ten splits of the tree (JMP 2012). Five-fold cross-validation was used to select the best models. The tree was pruned by examining the k-fold R^2 value. Smaller trees were preferred to provide simpler tree structures and variable relationships. This could potentially be determined with a cost complexity factor in the future, but here would be arbitrary. The column contributions were analyzed to determine which classifiers contributed the most to the reduction in the sum of squares error from tree formation.

Although it may seem like the regression tree analysis would have been better applied in the exploratory analysis because it created rules similar to what we are looking for, it required knowledge of which classifiers to consider. Furthermore, it can only split data into two groups at a time rather than multiple levels, and has the ability to split the same variable at multiple hierarchies. Thus, it provided useful information about classifiers that contribute to the variation, but cannot be used exclusively.

One way the regression trees were used in the exploratory part of the analysis was to identify which environmental midpoints were subject to data source error. Each midpoint was independently

considered as the dependent variable and data source was one of the predicting variables. If the data source contributed a large percentage to the sum of squares error, that environmental midpoint was removed from the analysis. These impacts were eliminated because data source does not provide an interesting analysis, but rather confounds the finding of more useful parameters.

2.3.3 Aggregation of Methods

Once the best classifiers were determined in each of the five methods described above, a frequency distribution was created. A classifier was evaluated for the number of times it was identified as a top classifier across the methods. Those that were recognized most frequently were selected as most promising for taxonomy formation and prediction.

2.4 Taxonomy Formation

The goal of the analysis was to create a more effective and efficient hierarchical materials classification structure. These terms are defined in the following ways:

Effectiveness: By providing more information, do I get closer to the actual impact of a given material? In addition, have I reduced the uncertainty in the groups that I will sample from to simulate a given process?

Efficiency: Does the information I am adding (i.e., each additional group) provide value, is it knowable, and how much information have I had to add?

The specific methods considered to address these questions are discussed in the following sections. These criteria were used to evaluate taxonomies and pick exemplary ones that seemed to perform well for these attributes.

2.4.1 Effectiveness

There are three parts to the discussion of effectiveness described above, which were previously referenced in Section 1.4.

1) How close is the "predicted" impact for a given material to its "true" impact, or in other words, what is the percent error from the individual database entry?
2) For what percentage of materials does the percent error decrease when more information is provided in the taxonomy?
3) What is the uncertainty of the proposed groups in the taxonomy, and how does it change as more information is provided?

To answer the first question, we considered how close the actual reported environmental impacts were to the predicted values, which here will be described as the median of the group of which a material is a part. By selecting the median, we can avoid distributional biases. The median absolute percent error (MEDAPE) was used to assess how close we are to the predicted impact, which is calculated using Equation 8:

$$MEDAPE = median\left(\frac{|x_{ij} - median(x_j)|}{x_{ij}}\right) \quad \text{(Eq 8)}$$

The MEDAPE allowed a calculation of the error normalized by the actual impact value, and so higher impact materials in the skewed distribution were not unduly represented due to large absolute deviations.

In response to the second question, for each material, we evaluated whether the deviation of the impact from the median impact of the group to which the material was assigned decreased by adding a level of information. For example, was the absolute percent error lower in level 2 than in level 1? This metric reported the percentage of materials for which the absolute percent error decreased with the proposed classification structure.

For the last question, typical metrics such as the coefficient of variation (COV, or the standard deviation divided by the mean) are often considered. However, the COV is best used to describe normal distributions. In this analysis, the groupings were not necessarily distributionally based and were often skewed, making this metric misleading. In lieu of the COV, the median absolute deviation coefficient of variation (MAD-COV) was evaluated. The MAD-COV is defined by Equation 9:

$$MAD - COV = \frac{median(|x_{ij} - median(x_j)|)}{median(x_j)} \quad \text{(Eq 9)}$$

The MAD-COV again used the median values to avoid challenges with distributional assumptions, but still provide a sense of the relative spread of the data. The MAD-COV allowed us to understand the variation within each group in the taxonomy. One caveat with MAD-COV is that it can increase with additional information when the uncertainty is captured within a smaller group. To accommodate this and to analyze the overall effect on a proposed structure, the weighted average MAD-COV for a proposed taxonomy was calculated. This MAD-COV for a given group was weighted by the number of elements in the group and then normalized by the total number of materials being analyzed.

Alternatively, the SSW/SST metric was also analyzed to gain an understanding of the residual uncertainty within the data. This provided slightly different information, as it emphasized the influence of outliers within the data. Thus, the SSW/SST helped us to understand how well we have accounted for the outliers within the taxonomy. This metric provided a number of benefits: it was easy to interpret, it represented error across the environmental profile, it did not require uncertainty assumptions, it penalized outliers which could be an indication of poor characterization, it was unsupervised and

required no external data, and similar methods were used by the clustering and regression tree algorithms to determine residual error.

Despite this range of metrics and the numerous metrics that were explored in the development of this work, these metrics remain non-optimal. They do not allow the selection of a "best structure", but rather permit the consideration of trade-offs in possible structures. More development may be needed in this space, and possible future metrics could include likelihood based metrics (although these may require distributional assumptions), hierarchical modeling assessments, or other algorithm development.

2.4.2 Efficiency

There are two parts considered for the efficiency discussion.

1) What is the "cost" of information required to identify where a material falls in the classification structure?
2) Are the groups created in a given level of the taxonomy distinct from other groups in that level, thereby demonstrating the value of the additional information and the ability to distinguish materials?

For the first question, the number of groups in a given structure was used as a proxy for the cost of information. In the future, cost could be determined based on the cost of collection for specific data. Actual cost was not included at this time, and may be dependent on the user. Choice of classifiers in this analysis was based more qualitatively on what expertise in LCA has indicated would be knowable, but in the future this would be better evaluated quantitatively, and may require more assessment of what information is readily available to potential users.

In response to the second question, we want to assess how much overlap there was between groups. This can be evaluated with the distinction rate. To calculate the distinction rate, elements of each group in a proposed classification were sampled via Monte Carlo simulation. The maximum percentage where one group had higher impacts than another was evaluated for all pairwise comparisons. The average value of these pairwise comparisons was the distinction rate. It is understood that this metric would be extremely high in the case where each database entry belonged to its own independent group. However, the distinction rate still does provide an inclination of whether groups add value relative to

other groups. Therefore, the distinction rate must be considered in conjunction with the number of groups to fully assess efficiency.

2.5 Streamlined Applications

Two examples of potential applications of the methodology developed in this thesis were demonstrated and will be described in Chapter 4. The first example showed how the proposed taxonomy can be used in under-specification. Three types of analyses using under-specification were performed; the first examined the effect of progressive information through the levels of the taxonomy, the second considered comparative analysis of two product alternatives using under-specified data, and the third calculated how many elements were present in the set of interest (SOI) at different levels of the taxonomy when applying probabilistic triage to under-specified data. The second application of the methodology demonstrated using identified classifiers to develop predictive models.

2.5.1 Under-Specification of Data

The demonstration of under-specification required a BOM of a fully specified product (i.e., each component was mapped to a single life cycle inventory database entry). Each of these components was then also mapped to all levels of the taxonomy based on appropriate classifier information. At a given level of specificity, Monte Carlo analysis was used to sample impact values from the subset of database entries that shared a group with the database entry specified for a given component. Simulation assured that only actual impact values were used and no distributional assumptions were required. Distributional assumptions were only applied at the individual database entry level, as there is some uncertainty even in the most specified data. Lognormal distributions were assumed for each data point, where the mean was based on the database entry's impact value and the standard deviation was chosen through a pedigree matrix approach using Equation 10:

$$\sigma_g^2 = exp^{\sqrt{[ln(U_1)]^2+[ln(U_2)]^2+[ln(U_3)]^2+[ln(U_4)]^2+[ln(U_5)]^2+[ln(U_6)]^2+[ln(U_7)]^2}} \qquad \text{(Eq 10)}$$

where U_i's are uncertainty factors based on reliability, completeness, temporal correlation, geographical correlation, other technological correlation, sample size, and other basic uncertainty (Frischknecht et al. 2007). For simplification, indicator scores, which are used to assign default uncertainty factors, that exist in databases, such as Ecoinvent, were ignored for this analysis. All indicator scores were set to three to assume a medium level of uncertainty. Monte Carlo simulation was used to generate 5000 samples.

2.5.1.1 Effectiveness at Different Levels of the Taxonomy

After sampling via Monte Carlo methods, the trial values were evaluated for their effectiveness. The same metrics as used for taxonomy development were considered for the example product as a whole: the MAD-COV at a given level of specificity and the MEDAPE. In lieu of using the median of an assigned group for the predicted value in the MEDAPE calculation, the value sampled at the most specified level (level 4) in the taxonomy was used.

2.5.1.2 Comparative Decision-Making with Under-specified Data

For the under-specification example demonstrating comparative analysis, the distinction rate was calculated to determine if the two products could be differentiated. Here the distinction rate involved only one pair of simulated values to compare: product A at level n and product B at level n.

2.5.1.3 Identification of the Set of Interest Using Probabilistic Triage

The SOI comprises the smallest group of components that represents the largest contributors to the overall environmental impact of the product, where this is evaluated at a certain percent contribution to the total and at a given confidence level. Probabilistic triage involved the use of the simulated values from the Monte Carlo analysis to identify this set of components, which were then to be further specified. Olivetti et al. developed this method for streamlining to create hybrids, where the SOI was specified at the database entry level (level 4 in this thesis) and the rest of the data were specified at the least specified level (level 1) (Olivetti et al. 2013). The SOI is evaluated via Equation 11:

$$SOI^{\xi} \subseteq \sum \left| P\left\{ \frac{I_{SOI}^{\xi}}{I_{\Sigma}^{\xi}} \geq T \right\} \geq C \right. \qquad \text{(Eq 11)}$$

where ξ is the level of specificity, I_{Σ} is the total impact, T is the threshold or percent contribution to the total impact desired, and C is the confidence level. SOI identification involved ranking components based on their average contribution to the total impact, and then identifying the set for which the threshold was exceeded at a given a given confidence level. For demonstration purposes in this thesis, the number of elements in the SOI was calculated at different levels of specificity, and the subsequent analysis using triaged hybrids was ignored. A threshold value of 75% and a confidence level of 90% were selected for the case study.

At level 4, confidence is very high about which components should be a part of the SOI, so this was deemed to be the "true" SOI. At levels 1 through 3, the number of components in the SOI was greater

than in level 4 due to higher uncertainty in the assessment, and therefore required specification of additional components beyond the true SOI. The additional percentage of components (APOC) that were required beyond the true SOI was calculated as per Equation 12:

$$APOC = \frac{SOI^{\xi} - SOI^{L4}}{n - SOI^{L4}} \quad \text{(Eq 12)}$$

where n is the number of components in the product, and SOI^{L4} is the number of components in the SOI at level 4, or the true SOI. The additional components were normalized in Equation 12, because the number of components in the true SOI differed across impacts.

2.5.2 Development of Predictive Models

In a second example of the methodology developed in the first part of Chapter 2, predictive models were created using the classifiers identified in the analysis. The models were generated via stepwise regression using the k-fold cross-validated R^2 values to assess the effectiveness. Five-fold cross-validation was performed in this analysis to make better use of the limited dataset. Other parameters such as the VIF, the p-values for explanatory variable significance, and residual normality were also evaluated.

The next section will demonstrate how the taxonomy creation methodology developed in this section was applied to different material types.

3 Application of Methodology – Materials Taxonomies

This methodology for developing hierarchical taxonomies has been applied to three material groups to explore how the approach performs with different material types. Any type of process dataset could be considered in this type of analysis, but materials were chosen as they are often upstream and outside the operational control of the party conducting the LCA. Thus, they represent an important area where significant data gaps occur and proxy selection is prevalent. The three groups explored here are metals, polymers, and precious metals. These materials make up a large portion of everyday products, and so are useful to explore. The materials were separated into material types (i.e., metals, polymers, and precious metals) prior to the analysis to ensure more uniformity within the data. It was assumed that materials of a given type might have more similarities in production and properties that might tend towards the identification of representative classifiers.

Each of these material groups represents a level 1 (most under-specified) category in the previous work by the author's research group (Patanavanich 2011). In this prior work, challenges were identified in determining intermediate levels between the most under-specified and the least under-specified levels (i.e., a specific database entry), which is level 4 here. The next sections look at the creation of two additional levels between those extremes, which here will be termed level 2 and level 3. The number of levels created is somewhat arbitrary, as there is a continuum between information and data uncertainty.

In creating the datasets, there were some challenges in identifying which materials to include and exclude, since it can be difficult to distinguish between upstream process data and material process data. Furthermore, as mentioned earlier, the boundaries are not the same across data sources and some material processes also include subsequent processing. In general, upstream processes that would not be used in a product have been excluded. However, there are a few exceptions to this, such as in the polymers dataset, where entries were included when processes only existed for the constituents used to create some of the thermoset materials. A list of all database entries is included in Appendix C for reference.

Each material group will be analyzed separately in this section, and in Chapter 5 will contain further discussion of the methodology as a whole.

3.1 Metals Taxonomies

3.1.1 Dataset Formation

Metals process data were collected from the sources listed in Sections 2.1.1 and 2.1.3. 168 database entries for metals were considered in the analysis after the above mentioned exclusions were made. A summary of the classifiers examined are listed in Table 3-1.

Table 3-1. Classifiers evaluated for the metals dataset

Classifier Category	Classifier
Characteristics of individual process datasets	Database source Recycled content Level of processing
Qualitative categorization of materials	Ferrous vs. non-ferrous Function Grouping in the CES database Toxicity classification
Materials properties	Price Density Tensile strength Relative crustal abundance Galvanic potential Melting temperature Commercial purity

The characteristics of individual process datasets were obtained from database documentation. The database source was included to ensure that any effects were not caused by the source of the data. As recycling significantly alters processing of metals from virgin extraction, recycled content was included as a factor. When it was not fully specified, recycled content was estimated based on process quantities, for example, by considering the amount of scrap included.

In terms of qualitative categorization, a breakdown based on ferrous vs. non-ferrous metals was examined, since it was the first classifier chosen within the previous work by this research group and therefore provided a baseline for comparison. Next, the function was considered, because the function of a material may be related to its environmental impact and also represents a knowable characteristic, since manufacturers may consider a set of substitutable materials or design alternatives. The function was determined by reading typical use descriptions in the CES database and making intuitive groupings based on these descriptions. Possible functions include: metals used in electronics, metals used in

energy products (e.g., batteries), metals used in structural applications, metals used in specialty or smaller quantity applications, and metals used in other bulk applications. A few combinations of these categories were considered in the subsequent analysis. As these categories are subjective, it is not always clear as to in which group certain materials would fall, e.g., should solder be included in the electronics group or with the specialty metals.

Since human health non carcinogenicity was one of the environmental impacts evaluated, relative toxicity of metals was considered as a classifier. A few classification systems for toxicity were found in literature; however, none of these proved effective with the metrics used nor were extensive enough to cover the entire set of metals. Furthermore, toxicity is not a well-defined criterion. Thus, toxicity has not been considered in this analysis, but may be a valuable contributor in future work with more exploration.

A few materials properties were included that might relate to environmental impacts. Some of these were identified through the exploratory analysis described in the next section. Properties included both fundamental properties (e.g., density) as well as emergent properties (e.g., price). The values for these properties were predominantly taken from the CES database when available, but supplemented from additional sources, such as for secondary metals (Recycle.net 2007a; City Chemical 2013; GSM Technology 2013). The values used are not necessarily precise, as the metals are described differently in the two databases, and translation between the two was a challenge. For instance, CES uses specific alloys, whereas this information is not supplied in process data documentation, and in fact the process data may be an aggregation of multiple alloys. Therefore values are meant to provide a relative sense of the performance of the classifiers rather than be exact. Price information is even less precise, as it is a dynamic parameter.

Relative crustal abundance was estimated by first determining an elemental composition of the dataset based on database documentation. In certain cases, this was calculated using stoichiometric mass ratios. The relative composition was then multiplied by the crustal abundance for each element to determine a relative crustal abundance, i.e., how much of the alloy is rarer and potentially more difficult to extract (Winter 2007). Although this will not directly translate to the ease of mining and relative ore concentrations for example, it can serve as a proxy for this information.

Originally, the goal was to consider all nine impacts within TRACI 2.0. However, upon examination of the first clustering iteration including all nine, it became apparent that the source of the data was very

important in determining the groupings. Although this result is useful for understanding process data as a whole, it can confound attempts to understand groupings based on other categorizations. Thus, regression trees were explored for each impact individually to understand which impacts were dominated by the data source. A number of classifiers were used as possible predictors and those where data source contributed 50% or more to the reduction in variation were eliminated from this study. As seen in Figure 3-1, five of the impacts (ecotoxicity, eutrophication, human health carcinogenicity, ozone depletion, and respiratory effects) were subject to this limitation, while the other four (acidification, global warming potential, human health non carcinogenicity, and smog formation) were not. As no good method of removing the data source error has been identified as of yet, the analysis proceeded with the smaller set of four impacts.[3] While these do not represent the full range of impacts desired, they do take into account unique aspects of a material's environmental profile and illustrate the application of the methodology in a multi-dimensional context. This set of impacts was used for all material categories in this thesis to create a consistent set of impacts around which to develop metrics.

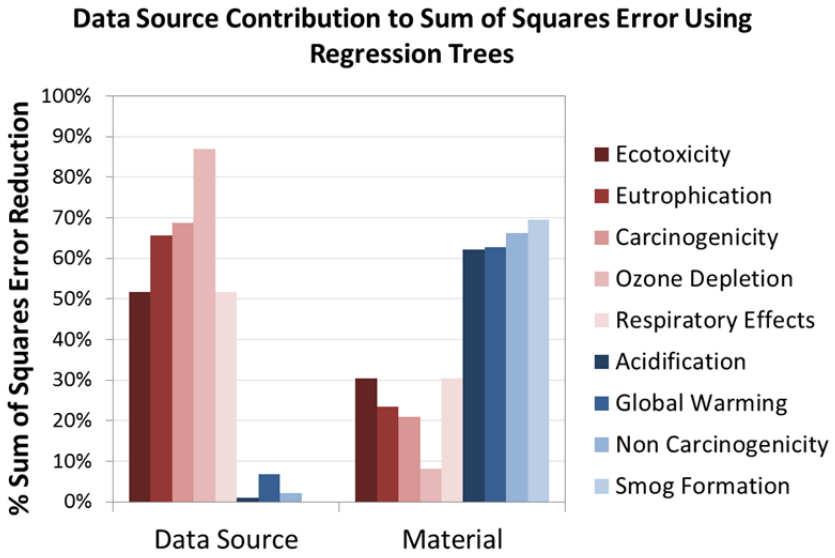

Figure 3-1. Relative contribution to sum of squares error using regression tree analysis from the two most significant classifiers: data source and material

[3] Some methods attempted to remove data source error included pairwise matching of data across databases and regression based correction methods.

3.1.2 Exploratory Analysis and Classifier Identification

Using this dataset, exploratory analysis was performed to examine the underlying patterns in the data. First, visualization of the data highlighted the skewed nature and the presence of a number of significant outliers, which can be seen in the boxplot in Figure 3-2. A few outliers and influential points are indicated on the chart, and each of these was confirmed as an outlier using the Mahalanobis distance test for all four impacts.

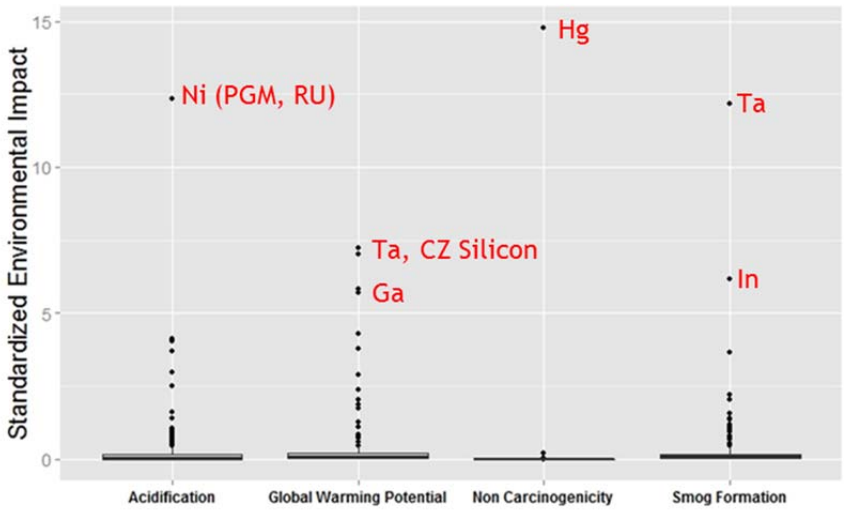

Figure 3-2. Boxplot of standardized environmental impacts for metals with some outliers and influential points identified. Materials identified include: Ni (PGM, RU) = Nickel from platinum group metal production in Russia; Ta = Tantalum; CZ Silicon = CZ single crystalline silicone, electronics grade; Ga = Gallium; Hg = Mercury; and In = Indium.

PCA was also performed on the dataset and the same set of points was identified, and can be seen in Figure 3-3. It is interesting to note that non carcinogenicity is contrasted to all of the other impacts, thus explaining a unique portion of the variation in the data. However, only one influential point lies along this axis, indicating that the relative variation in non carcinogenicity is dominated by mercury.

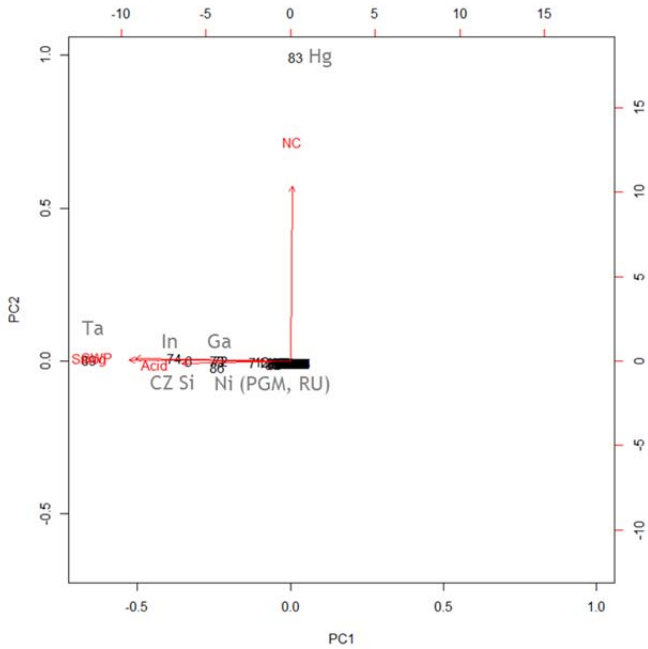

Figure 3-3. Principal component analysis on the metals dataset with influential points indicated. Plot shows principal component 1 versus principal component 2.[4]

Lastly, clustering analysis was conducted using the Ward method. Upon examining the knee of the joining distance scree plot, 14 clusters were evident. However, if the plot was examined for where the greatest distance gains had been achieved, a smaller set of six clusters was selected. Examination of just these six clusters for the first tier analysis provided the information in Table 3-2. The environmental profiles of the clusters can be seen in Figure 3-4. Figure 3-4 is broken into six plots, each of which represents a cluster of material processes, where a line in the plot shows the impacts for a single process. The relative values for each of the four impacts are shown on the vertical axis. Cluster 1 has a lot of variation within the set of materials, particularly for global warming potential, whereas cluster 2 is comprised of all of the metals that have relatively low values across all impacts. The other clusters are unique because of their impacts in a given category. Clusters 4 and 5 seem somewhat similar to one another across impacts, which makes sense since both are comprised of expensive electronics materials.

[4] Acid = acidification, GWP = global warming potential, NC = non carcinogenicity, smog = smog formation

Table 3-2. Summary of metals clusters at level 2

Cluster #	Cluster Name	Cluster Description	Example Database Entries
1	Performance Metals	Includes some metals used in electronics products, energy products, and other high impact metals	Silicon, electronic grade Lithium Magnesium Soft solder, Sn97Cu3
2	Bulk Metals	Includes cheaper metals used in common construction as well as some other metals	Aluminum sheet Steel cold rolled coil Zinc sheet Lead, primary
3	Mercury	Only includes one material	Mercury
4	Expensive Electronic Metals	More expensive electronic materials	CZ single crystalline silicon, electronics Gallium Indium
5	Tantalum	Only includes one material	Tantalum
6	Nickel from PGM production in Russia	Only includes one material	Nickel from PGM in Russia

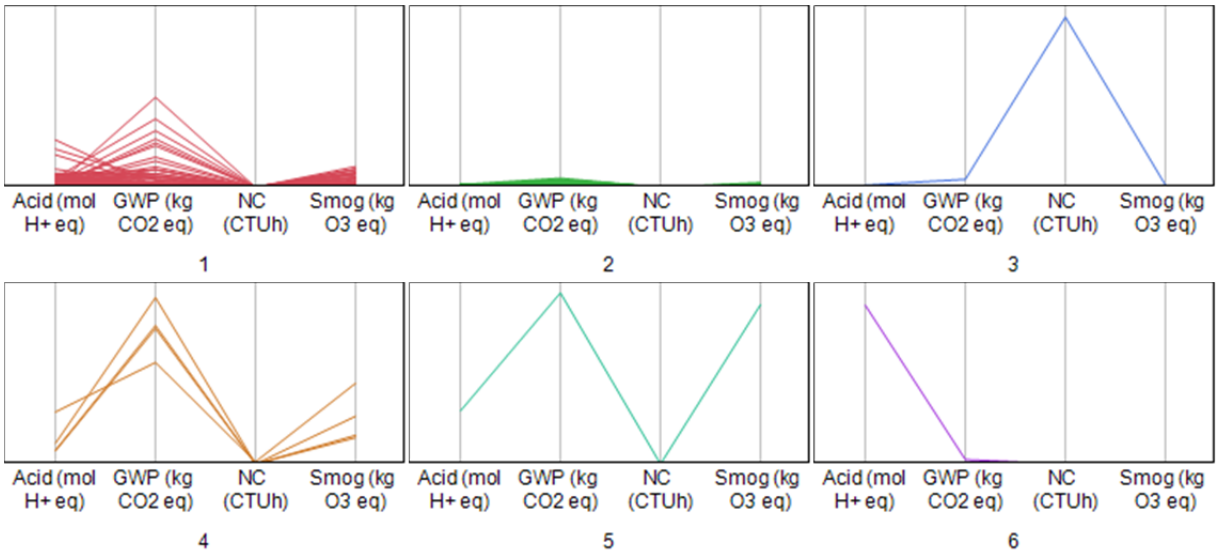

Figure 3-4. Environmental impacts of metals in each cluster by cluster number

From the cluster and PCA analyses conducted, a few key classifiers stand out as potentially viable descriptors of the groups that were created. The first is price: in general, higher priced items have higher environmental impacts and are segregated into their own clusters, whereas lower priced items form their own cluster as well. This effect is evidenced in Figure 3-5, which shows a fairly clear distinction between clusters based on price. The second key potential classifier is function: the

materials that have been highlighted as influential are typically used in electronics applications, whereas the lower impact materials are more commonly in structural or bulk applications. Although this analysis selected six clusters, if more splits are considered in the dendrogram, then other factors may be important as well. Observation showed some possible classifiers for future levels could be recycled content, ferrous vs. non-ferrous metals, and certain material groups that have distinct impacts, such as magnesium or tin based compounds. Lastly, the analysis indicated that two of the materials were significant outliers and needed to be segregated into their own groups, since they would significantly affect the variation of any group of which they were a part. One of these materials is mercury, and the other is nickel from platinum group metal production in Russia. The first makes intuitive sense, since mercury is known to be highly toxic. On the other hand, the nickel database entry should be explored further.

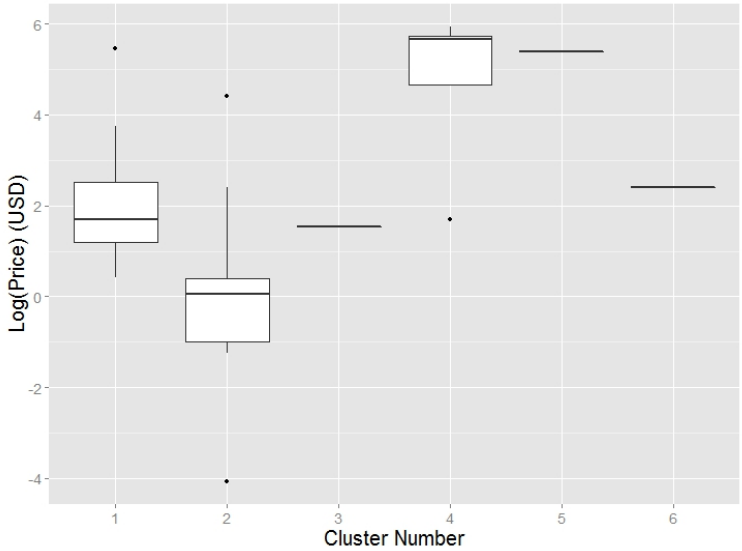

Figure 3-5. Price by cluster number for metals data. The boxplots are characterized by the median in the center, the first and third quartiles as the bottom and top of the box respectively, and the dots represent points that are more than 1.5 * IQR (interquartile range) from the quartiles. Clusters 3, 5, and 6 appear as lines since they contain only one element.

3.1.3 Classifier Evaluation

Each of the five metrics described in Section 2.3 Table 2-1 was applied to the metals dataset to understand which classifiers might be useful to explore both from an uncertainty and a modeling perspective. They are each documented here with supplemental information included in Appendix A.

PCA demonstrated that the logarithm of price was most highly correlated with the first PC (r=-0.74), and recycled content was correlated to a lesser degree (r=0.54). Recycled content has a lower correlation because of the wide range of metals with very low recycled content. The trend of recycled content as a significant classifier is most evident for materials with higher than approximately 25% recycled content. Density and crustal abundance were aligned with the additional uncertainty found in PC2. Upon examining boxplots of categorical classifiers, it was found that there was distinction between the groups for both function and ferrous vs. non-ferrous based on PC1. An example of one function categorization is shown in Appendix A, but was true for other permutations as well, such as when only electronics were considered. Less distinction occurred with additional function categories included, and so electronics and structural materials may be the functions that merit application.

Using the SSW/SST metric, a few groupings were able to significantly decrease the overall uncertainty across environmental impacts. Grouping based on price showed the biggest change, where the data were split into three parts for a 55% reduction as compared to the whole dataset. The best performance using price as a classifier was seen for smog formation and acidification. Recycled content and function showed 45% improvement in the overall uncertainty. All proposed categorizations showed the least improvement in global warming potential.

All of the logistic regression models exhibited significant predictive capabilities. The best logistic regression models were able to show approximately 15-25% misclassification rates on the validation data. However, given that some categories made up a large percentage of the data, this represented approximately a 45-75% improvement over the baseline. The best performing model in terms of validation data was based on crustal abundance, which showed a higher percent correct than for the training model. The density and price validation percentages showed similar performance to the training models. The function model that only included electronics performed well on a percent misclassification basis, but given the large number in the baseline, very poorly on percent improvement. One function model that included groups for both structural materials and electronics materials did perform better on this metric.

A fairly good linear regression model with an R^2 equal to 0.76 was generated. Price and recycled content were very significant, and relative crustal abundance and data source made up some of the residual uncertainty. There is some residual variation, so either some error remains from the data source that we cannot fully account for or other classifiers are required. The parameters chosen

performed the best on the validation data, and all were shown to be significant with little multicollinearity as demonstrated by the VIF values. The residuals approximate a normal distribution, with some deviations at the tails.

Lastly, the pruned regression trees with only five splits showed that recycled content and price were the main factors of importance contributing to the reduction of sum of squares error. Additional pruning left a simplified hierarchical prediction of the overall environmental impact. This showed that first, very low recycled content materials should be segregated (this can be seen as the group with great spread in the PCA plot). Then within each of those groups, different price point threshold values were relevant. The simplified pruned regression tree is shown in Figure 3-6.

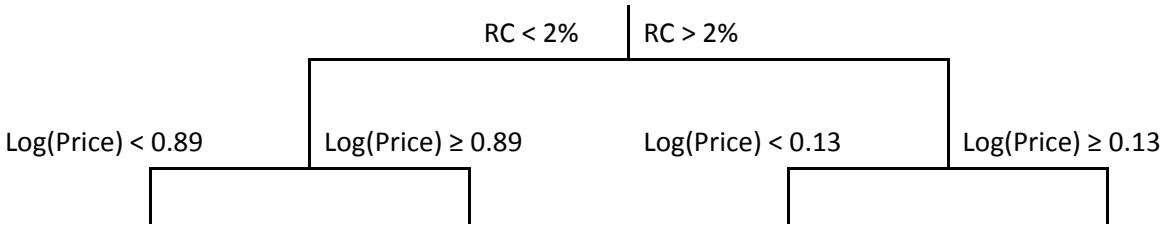

Figure 3-6. Regression tree for metals showing splits based on recycled content and log(price)

Table 3-3 shows the aggregated summary of the classifiers which are important in each of the methods described above. As indicated previously, more classifiers were considered in the analysis, but this subset contains the ones that continued to be relevant. Price appeared within every method evaluated. Other potentially significant classifiers included recycled content, function, and relative crustal abundance. Therefore, these classifiers may be important for application of taxonomies and/or for predictive algorithms. The baseline categorization of ferrous vs. non-ferrous does not seem to account for much of the variation in the data.

Table 3-3. Aggregated results of classifier evaluation for the metals dataset

	Ferrous/Non-Ferrous	Data Source	Recycled Content	Price	Function	Density	Crustal Abundance
PCA	x		x	x	x	x	x
SSW/SST			x	x	x		
Logistic Regression				x	x	x	x
Linear Regression		x	x	x			x
Regression Trees			x	x			

3.1.4 Taxonomy Formation

Based on the previous analysis, four main types of taxonomies were examined:

1) Baseline: ferrous vs. non-ferrous
2) Function based
3) Price based
4) Recycled content based

The specific groupings analyzed are shown in Table 3-4. The threshold values to break continuous classifiers into categories were selected either through regression tree analysis or qualitative examination of the boxplots. Each proposed level 2 taxonomy included the groups listed in Table 3-4 as well as a group for the mercury outlier and one for the nickel outlier.

Table 3-4. Summary of metals level 2 proposed taxonomies

Baseline	Function			Recycled Content	Price ($/lb.)	
F/NF	F1	F2	F3	RC	P1	P2
Ferrous Non-Ferrous	Electronics Other	Electronics Structural Other	Bulk Electronics Energy Specialty Structural	A: < 2% B: ≥ 2%	A: ≤ 0.60 B: 0.60<P≤5.15 C: > 5.15	A: ≤ 5.15 B: 5.15<P≤148 C: > 148

These seven taxonomies were evaluated on the four metrics for effectiveness (median absolute percent error, percentage of materials with reduced error from level 1, and residual uncertainty via SSW/SST and MAD-COV) and the two metrics for efficiency (number of groups and distinction rate). The MEDAPE values for level 1 and all of the level 2 taxonomies are shown in Figure 3-7.

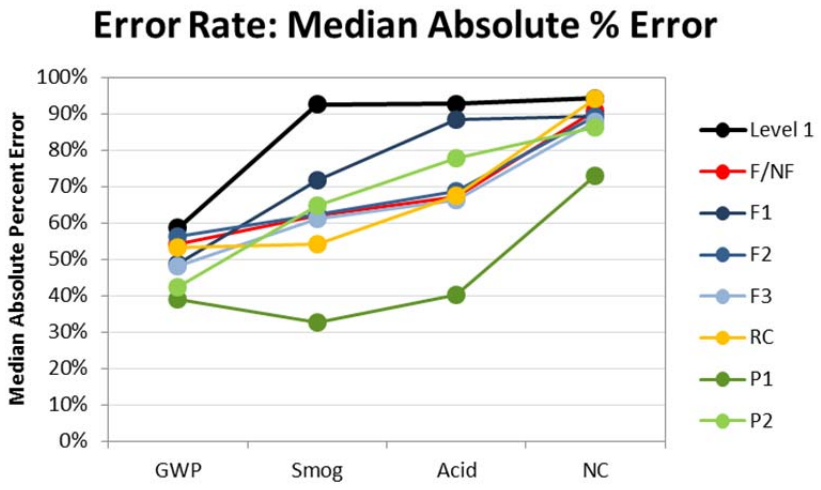

Figure 3-7. MEDAPE for level 1 metals and level 2 metals proposed taxonomies

Initially, at level 1, MEDAPEs for every impact except global warming potential exceeded 90%. The taxonomies were able to show improvement and in some cases significantly reduce the percent error. This was especially true for smog and acidification; P1 reduced the error by more than 50% in these cases. Non carcinogenicity remained the worst performing for all taxonomies. P1 performed the best on this metric, while many others were fairly comparable to one another, although higher than P1. P1 reduced the average MEDAPE from 85% to 46%, which is a significant improvement in estimation of impacts.

If we consider the percentage of materials for which we were able to improve our estimate of the impacts from level 1 to level 2, we see in Figure 3-8 that approximately two thirds of the materials are better off in the level 2 taxonomy. Although, this is not as high as would be desired, it is still some improvement. P1 tended to perform better than the other classifications, but the difference was small. The F1 categorization is one of the lowest in every impact.

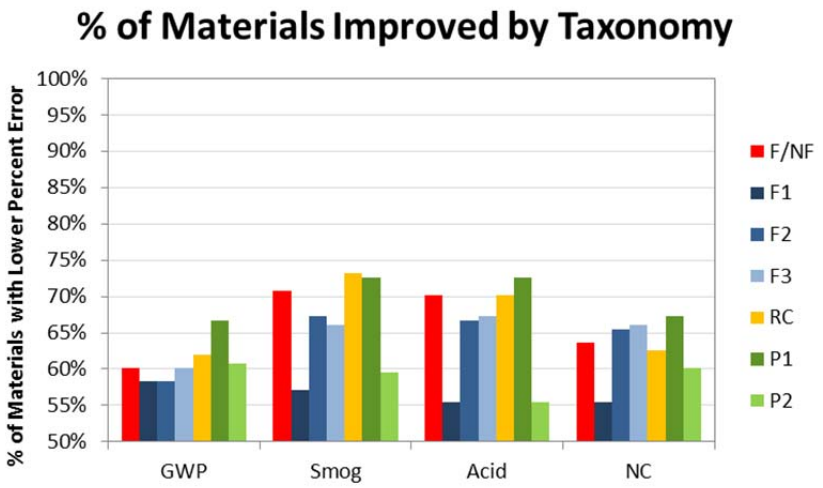

Figure 3-8. Percent of metals for which the percent error was less in level 2 proposed taxonomies

For the SSW/SST, we see in Figure 3-9 that P2 had the lowest values across impacts. This makes sense, since P2 was specifically designed to account for outliers by having a group for "high" and "higher" priced materials unlike P1. Ferrous vs. non-ferrous and recycled content are rather poor at segregating the outliers and do not account for most of the variability in the data. This plot shows further confirmation that mercury dominated the uncertainty for non carcinogenicity, since all proposed classification structures exhibited a very low SSW/SST for this impact simply by having a separate group for mercury.

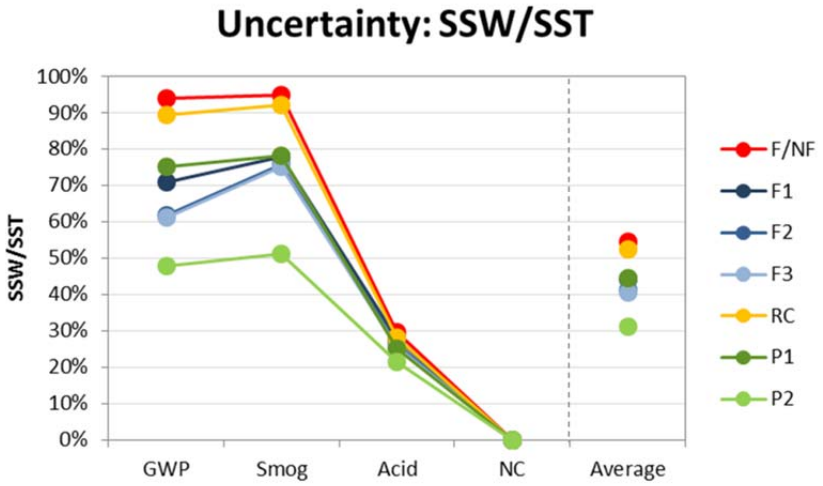

Figure 3-9. SSW/SST for level 2 metals proposed taxonomies

Lastly, if we look at the residual uncertainty present in the data through the MAD-COV metric in Figure 3-10, we see similar overall results. Many of the individual groups in a given taxonomy had a higher

MAD-COV than the dataset as a whole. This happened when high uncertainty was left in a group. A few examples are the global warming potential of non-ferrous metals and the electronics metals. Non-ferrous metals had a high level of uncertainty within the group, since only lower impact materials have been segregated out. Thus, this structure did very well at reducing uncertainty for the lower group, but very poorly for the rest (and majority) of the materials. This effect may be more clearly visualized using bubble plots for the MAD-COV, which are shown in Appendix B. For electronics materials, while many have a high global warming potential, there are a few with lower values that increased the spread in the data. When these were weighted by the number of elements in each of the groups, improvement was seen, since only a limited set of materials had higher uncertainty. In general, as more function categories were added, a few groups exceeded the baseline MAD-COV, although the weighted average decreased. Overall, price appears to have the highest effectiveness, both from the standpoint of having most groups below the level 1 MAD-COV and for having the lowest weighted MAD-COV.

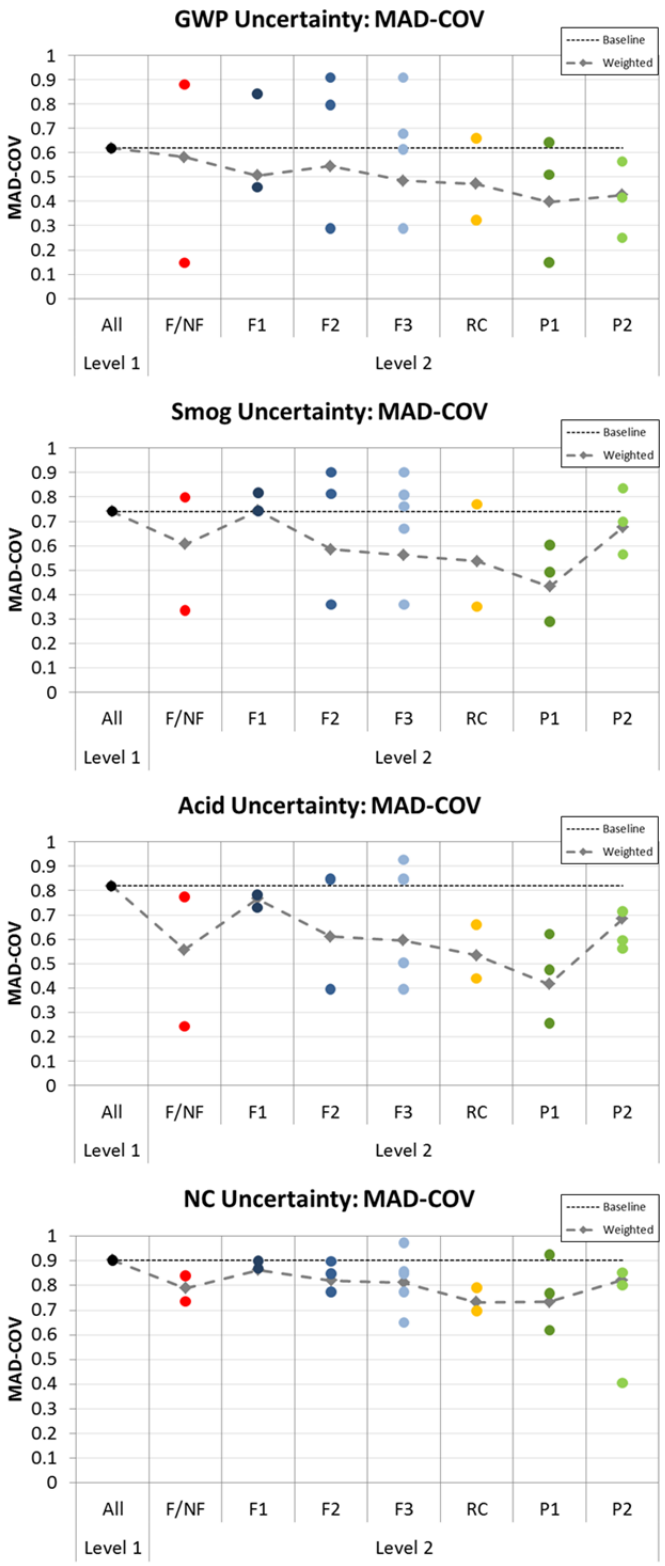

Figure 3-10. MAD-COV values by group within each proposed level 2 metals taxonomy. The black dashed line represents the baseline value set by level 1. The grey diamonds show the weighted average MAD-COV for each proposed taxonomy. Groups with a single element and MAD-COV of zero have been removed.

In terms of efficiency, the number of groups in each categorization is shown in Table 3-5 and the distinction rate is in Figure 3-11. Most of the structures had a relatively similar number of groups. Again some of the best performance came from price, with an average number of groups, but a higher ability to distinguish amongst those groups, particularly for global warming potential and smog. Thus, overall, price is the preferred choice: it has the highest effectiveness and the highest average distinction rate. However, one challenge with price is that the exact threshold values are difficult to determine. P1 split off the high and low price groups whereas P2 split off the high and higher price groups. Both show benefits on the effectiveness measures. The former achieved better error rates overall and the latter accounted for outliers better. Thus, it can be difficult to say which is the "best" taxonomy, and more exploration may be required optimize this structure.

Table 3-5. Number of groups in each level 2 metals proposed taxonomy

	F/NF	F1	F2	F3	RC	P1	P2
Number of Groups	4	4	5	6	4	5	5

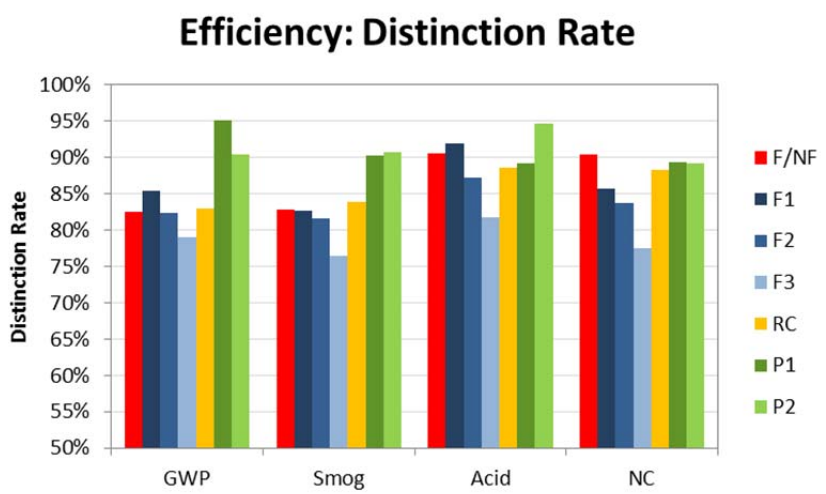

Figure 3-11. Distinction rate for level 2 metals proposed taxonomies

Ferrous vs. non-ferrous classification showed high efficiency by forming the fewest groups and by exhibiting a reasonably high ability to distinguish between them. This came at the cost of effectiveness however. If we look at the distributions of the values, we can see that the ferrous metals had very low values across all impacts, whereas there was a large spread in the non-ferrous metals. One example of

this is demonstrated for global warming potential in Figure 3-12. Thus, this is an effective taxonomy for splitting off low impact materials, but does little to account for most of the variability within the data.

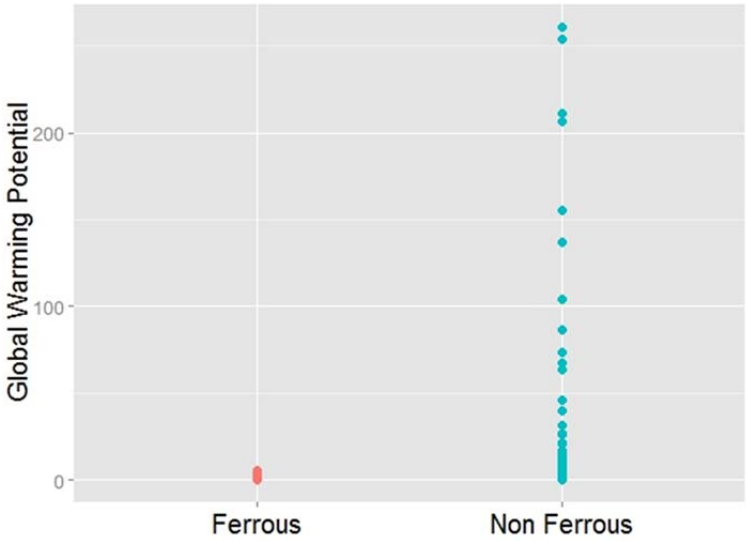

Figure 3-12. Distribution of points for the ferrous vs. non-ferrous categorization for global warming potential

Recycled content is similar to the ferrous vs. non-ferrous metals categorization in that it had higher efficiency and lower effectiveness compared to the other proposed taxonomies. However, it does slightly improve on effectiveness compared to ferrous vs. non-ferrous in most cases. Likely, classification based on recycled content is a useful subsequent level or additional piece of information, but does not form an effective categorization on its own. Similar to the ferrous vs. non-ferrous, it split off the low impact data as well, and left high variability in the rest of the data. There is some overlap in these classifiers based on available data.

With function, as more groups were added, the ability to tell them apart diminished, which earlier was shown by overlap in the boxplots for those groups. Thus, there was a decreased efficiency with little gain in effectiveness. A moderate selection would be to choose the intermediate function categorization that, similar to price, segregated the low and high impact metals.

3.1.5 Next Tier Analysis

As price was determined to be the best classifier based on the previous analysis, breaking up the data using the P1 classification was selected for a second tier of analysis. This included clustering on each of the subgroups (i.e., A, B, and C) to identify potential new classifiers to subdivide the groups. The number of clusters was determined at the point where the largest gains had been realized in the joining

distance scree plot. The results of the clustering analysis are shown in Table 3-6, Figure 3-13, Figure 3-14, and Figure 3-15.

Table 3-6. L3 cluster descriptions for metals categories P1-A, P1-B, and P1-C

Cluster #	Cluster Name	Cluster Description	Example Database Entries
A1	Low price-high NC	Includes 3 materials	Cast iron Steel, electric, un- and low-alloyed
A2	High recycled content	Mostly non stainless steels with recycled content >50%	Steel hot rolled coil Steel billet
A3	Low recycled content	Mostly non stainless steels with recycled content <50%	Steel sheet Steel cold rolled coil
A4	Al secondary 1	Secondary Al and one other	Aluminum, secondary, shape casted Cadmium sulphide
A5	Al secondary 2	Only includes one material	Aluminum, secondary, rolled
B1	Bulk metals	Includes other mid-priced metals	Aluminum sheet Stainless steel cold rolled coil Zinc sheet Lead, primary
B2	Magnesium	Magnesium and alloys	Magnesium Magnesium alloy AZ91
B3	High Smog Copper	Mix of copper, antimony, magnesium	Copper, SX-EW Copper from North America
B4	High Acidification Copper	Copper from certain mines	Copper from PGM in Russia Copper from Indonesia
C1	Performance Metals	Includes some metals used in electronics products, energy products, and other high impact metals	Silicon, solar grade Lithium Cobalt Soft solder, Sn97Cu3
C2	Nickel 99.5%	Only includes one material	Nickel, 99.5%
C3	Gallium	Gallium and one silicon	Gallium CZ single crystalline Si, electronics
C4	Tantalum	Only includes one material	Tantalum
C5	Indium	Only includes one material	Indium

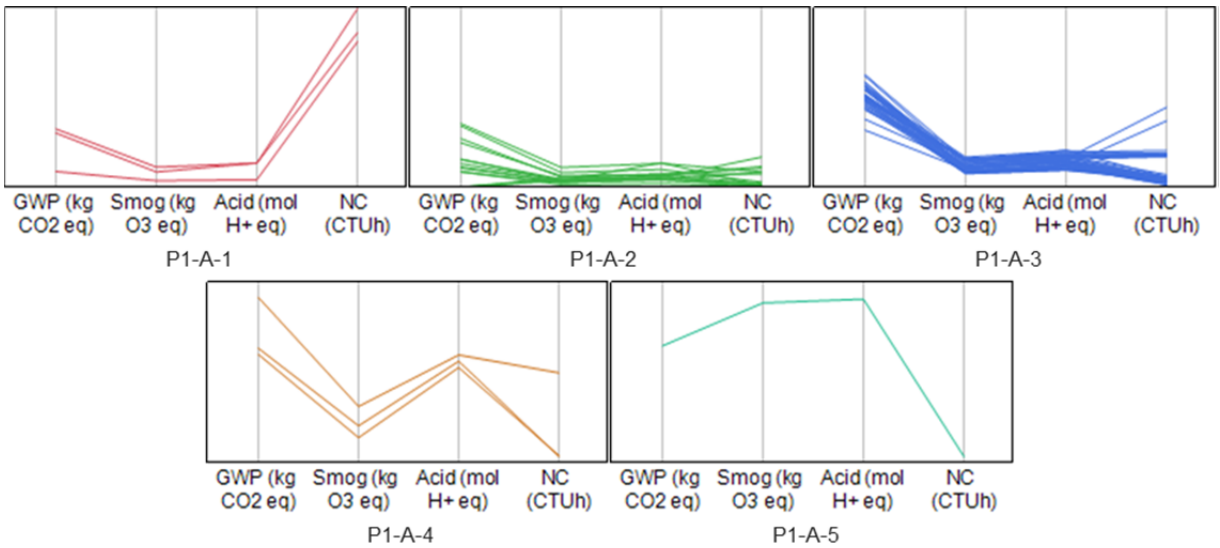

Figure 3-13. Level 3 clusters for metals category P1-A

The main factor differentiating the low-priced materials clusters was recycled content. Although most of the aluminum is in group B, the secondary aluminum has a lower impact and a lower price and ended up in group A. Clustering of P1-A formed two groups with secondary aluminum (A4 and A5), and so a group was formed for this material type. For the remainder of the materials in group A (mostly non chromium steels), the materials were separated by the recycled content, i.e., whether it was greater or less than 50%. This split is represented by clusters A2 and A3.

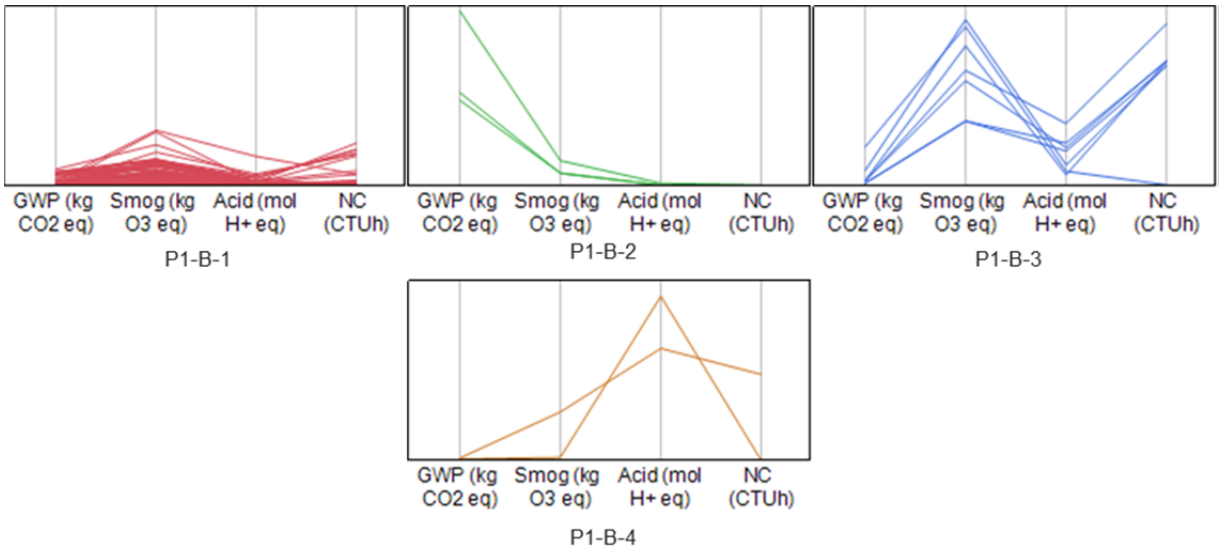

Figure 3-14. Level 3 clusters for metals category P1-B

Cluster B1 had a group of low impact materials, and the other clusters had a very high relative impact in at least one of the environmental parameters considered. Thus to reduce variability, these high impact materials were segregated. Unfortunately, insufficient information existed to understand the differences in the copper processes on a macro level, so all copper was combined, despite the formation of multiple copper clusters. It is understood that this will increase the variability in the assessment. Magnesium was also segregated due to its relatively higher global warming potential as compared to the other materials in group B.

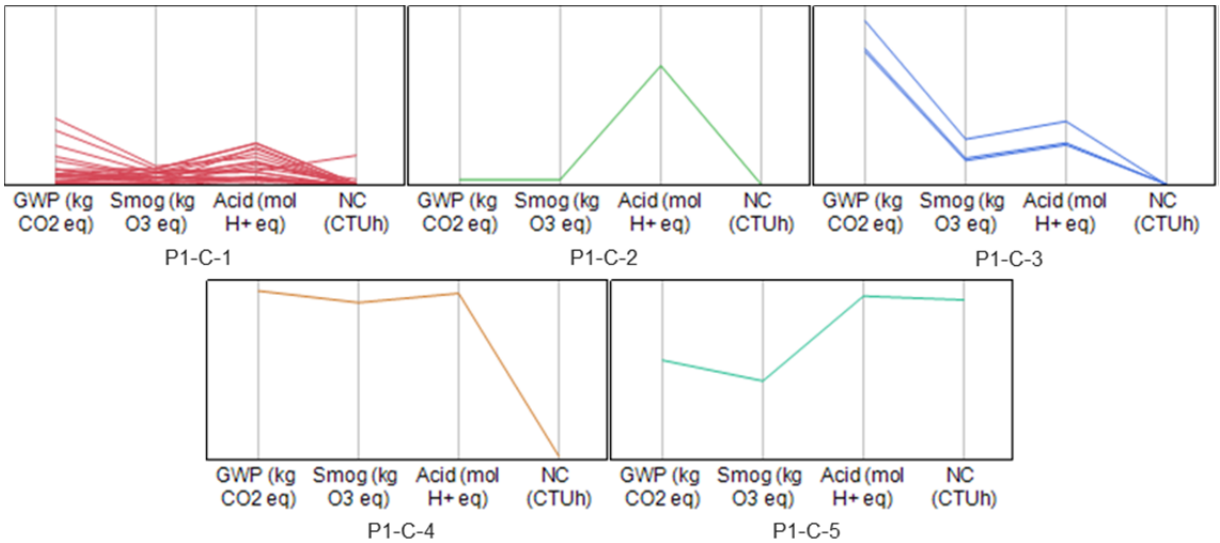

Figure 3-15. Level 3 clusters for metals category P1-C

Group C had more variability and higher impact materials. Insufficient information existed to segregate either the silicon or the nickel database entries that clustered separately from other similar database entries. However, the tantalum, indium, and gallium were isolated. A summary of the resulting final proposed hierarchical structure can be seen in Figure 3-16.

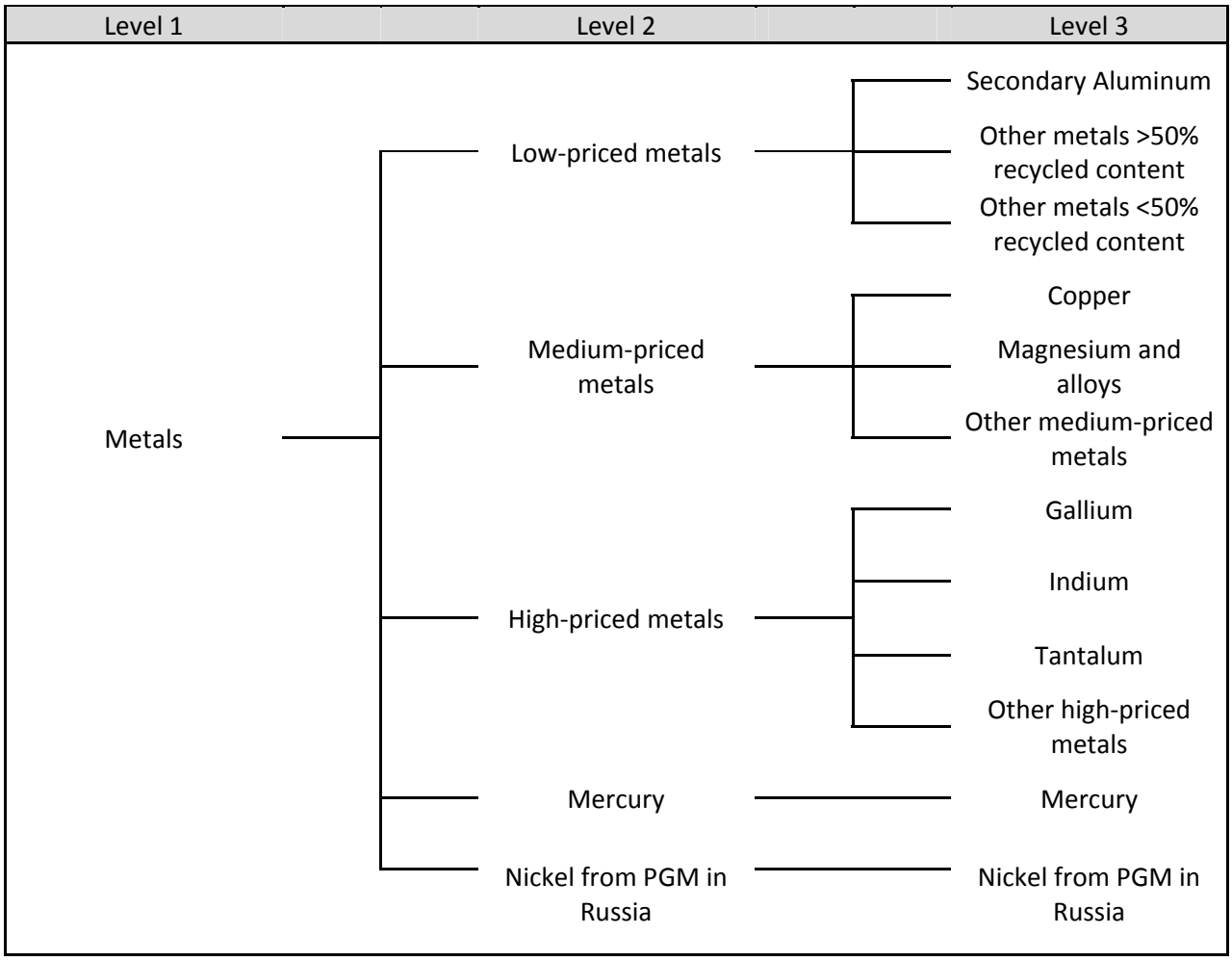

Figure 3-16. Proposed level 2 and level 3 hierarchy for metals

This next level in the hierarchy had 12 categories instead of the five for level 2. The additional categories reduced the average median absolute percent error across all impacts from 46% to 41% as seen in Figure 3-17. Furthermore, the average SSW/SST across all impacts dropped from 45% to 12%, shown in Figure 3-18. Considering uncertainty in terms of MAD-COV in Figure 3-19, we see that some of these groups are poorly characterized. In particular, the copper has a higher MAD-COV for all impacts except global warming potential and the other medium-priced materials in cluster B have a higher MAD-COV in global warming potential. In general, the weighted MAD-COV does decrease though. However, despite reducing the magnitude of the error, the error rate did not improve for a large number of materials from level 2 to level 3. Only 56-57% of materials improved on this metric. This indicates that the structure is performing better only for a subset of the materials present. Depending on the needs of the user, the effectiveness gains may be insufficient to justify the lack of efficiency due to providing

additional information. There was efficiency in distinction between categories however, as demonstrated by distinction rates of 90-94%. Thus, the categories chosen add some value, but at the trade-off of information cost.

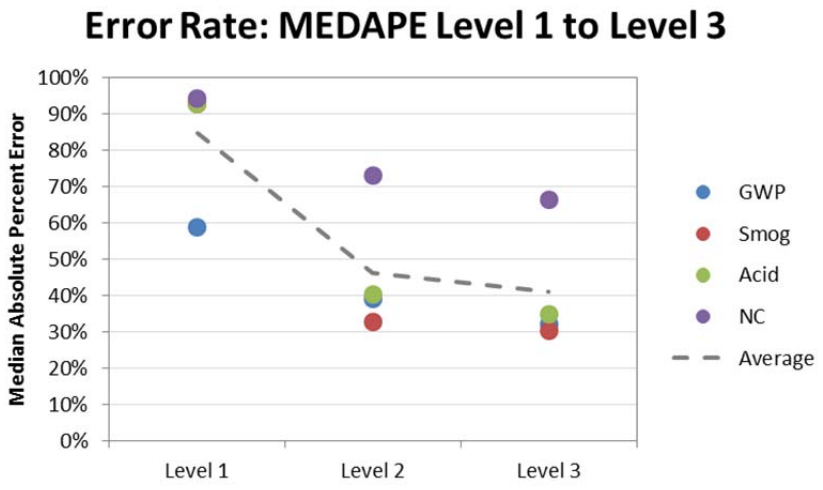

Figure 3-17. MEDAPE for metals from level 1 to level 3

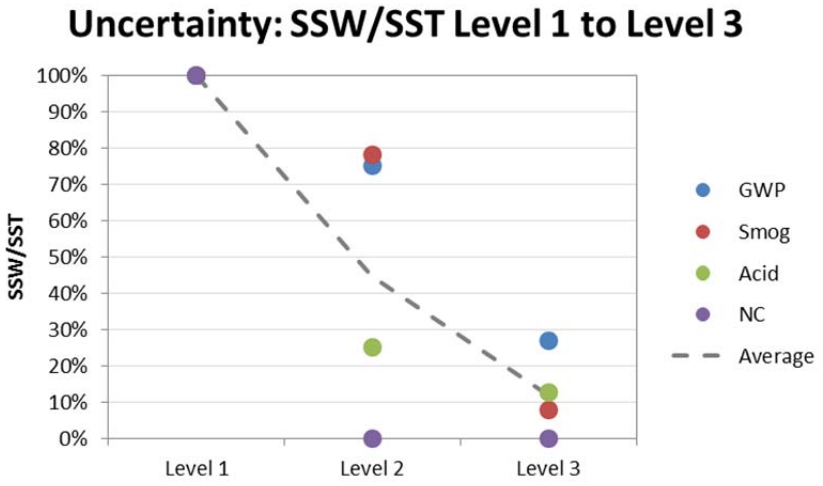

Figure 3-18. SSW/SST for metals from level 1 to level 3

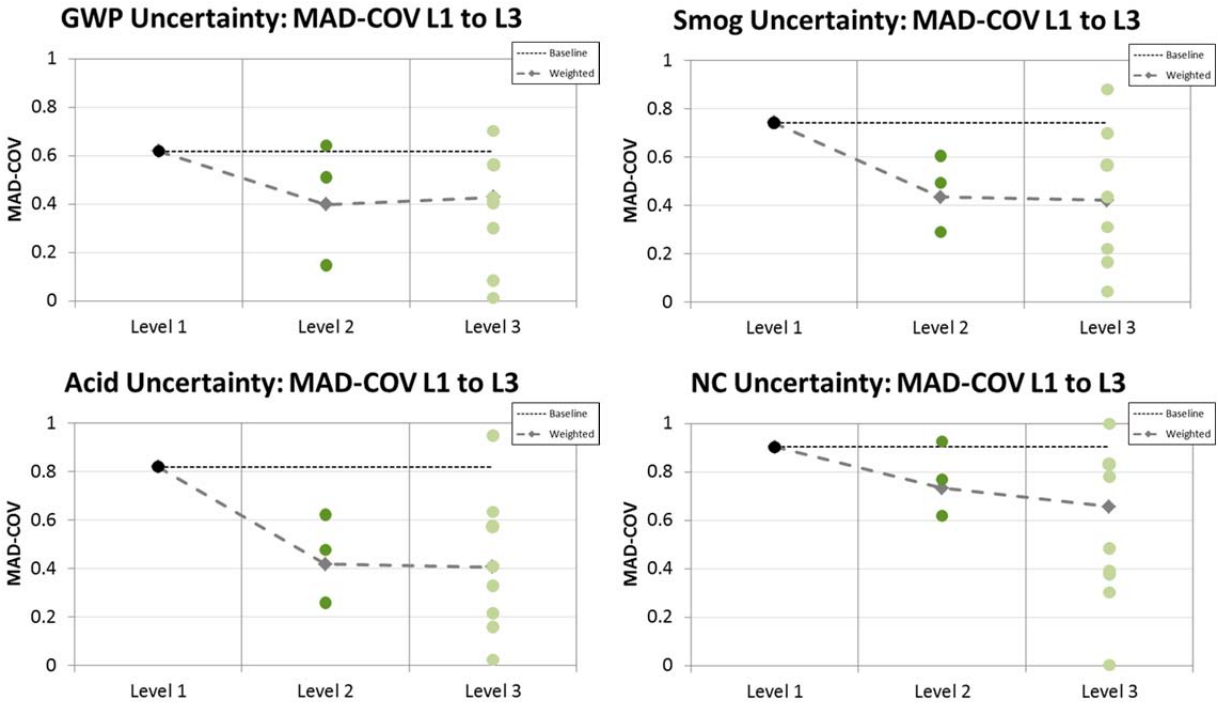

Figure 3-19. MAD-COV from level 1 to level 3 for P1 and then P1 subcategories. The black dashed line represents the baseline value set by level 1. The grey diamonds show the weighted average MAD-COV for each proposed taxonomy. Groups with a single element and MAD-COV of zero have been removed.

Taxonomy formation at level 3 may require some additional considerations. For instance, there may be a path dependency where a different previous level 2 classification could achieve even better results here through intuitive categorization. Furthermore, as seen across the copper processes, more details about individual processes may be required to successfully group materials at these levels. Lastly, since large error reduction was achieved between level 1 and 2, level 3 adds less value than the preliminary split.

While we see little improvement from level 2 to level 3, there is theoretically a point with further improvement prior to the database entry level. As a means of illustration, this hypothesis was explored for the copper cluster only, due to high uncertainty in that group. Clustering the copper group showed four clusters displayed in Figure 3-20. These clusters may be process based (i.e., mine location, processing method) or data source based (i.e., boundary assumptions, recycling credit assumptions). There was insufficient information in documentation of the datasets to fully discern the differences between the processes. The clusters showed a subset of the data that was higher only in global warming potential (cluster 2), one only higher in acidification (cluster 3), and one higher in most

impacts, with some variability (cluster 4). In lieu of forming intuitive clusters here, these four clusters were used as is, assuming that a theoretical classifier exists.

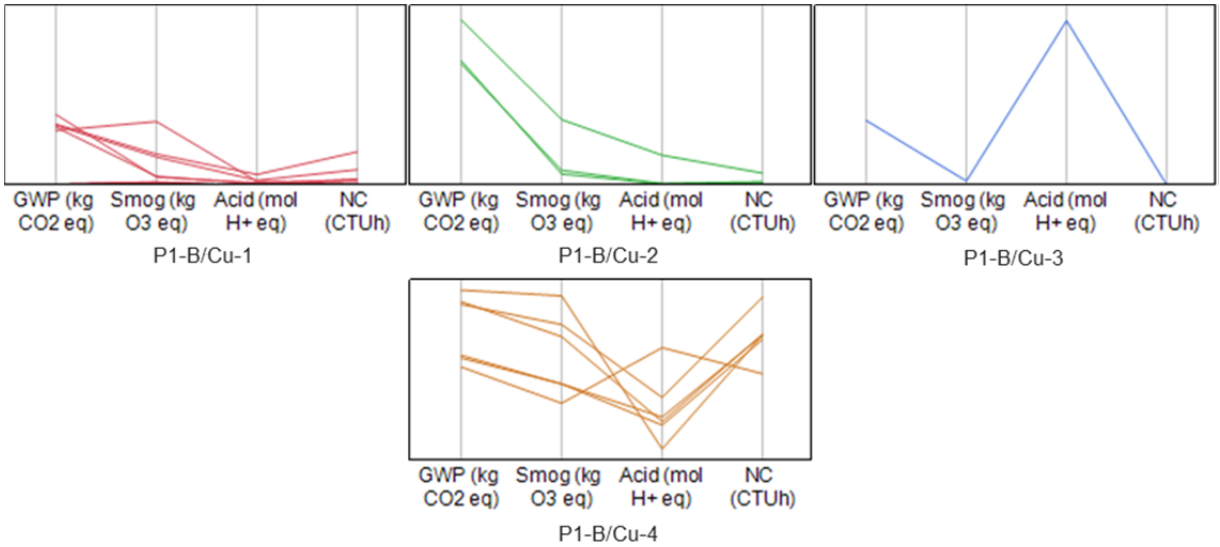

Figure 3-20. "Level 3+" categories for copper cluster from P1-B

As is, these clusters showed a reasonable improvement in the metrics analyzed. This can be seen in Figure 3-21, Figure 3-22, and Figure 3-23. The SSW/SST was reduced by an average of 79% from the copper group as a whole. The average MEDAPE of 75% for the copper group was relatively high compared to the rest of the data in level 3. However, with the four clusters, it was reduced to 33%. Lastly, the weighted average MAD-COVs for the clustered copper were approximately 45% or more below the MAD-COV for the copper as a whole.

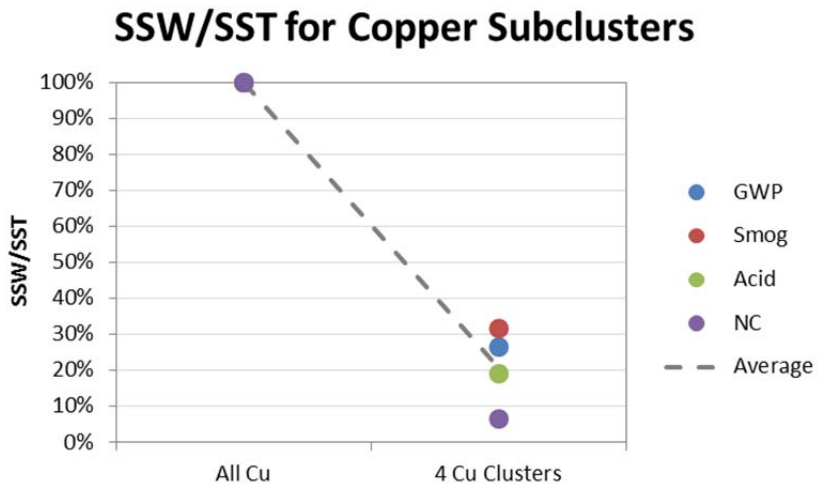

Figure 3-21. SSW/SST using all copper processes as the baseline and then after splitting into four clusters

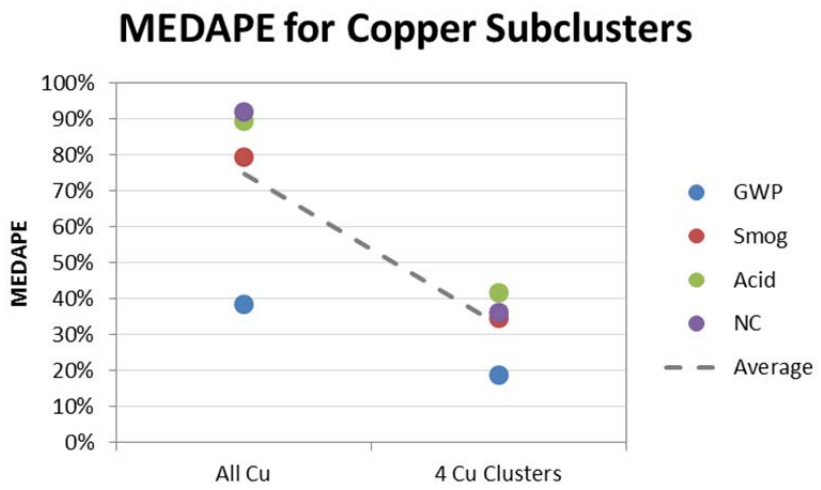

Figure 3-22. MEDAPE for all copper processes together and then after splitting into four clusters

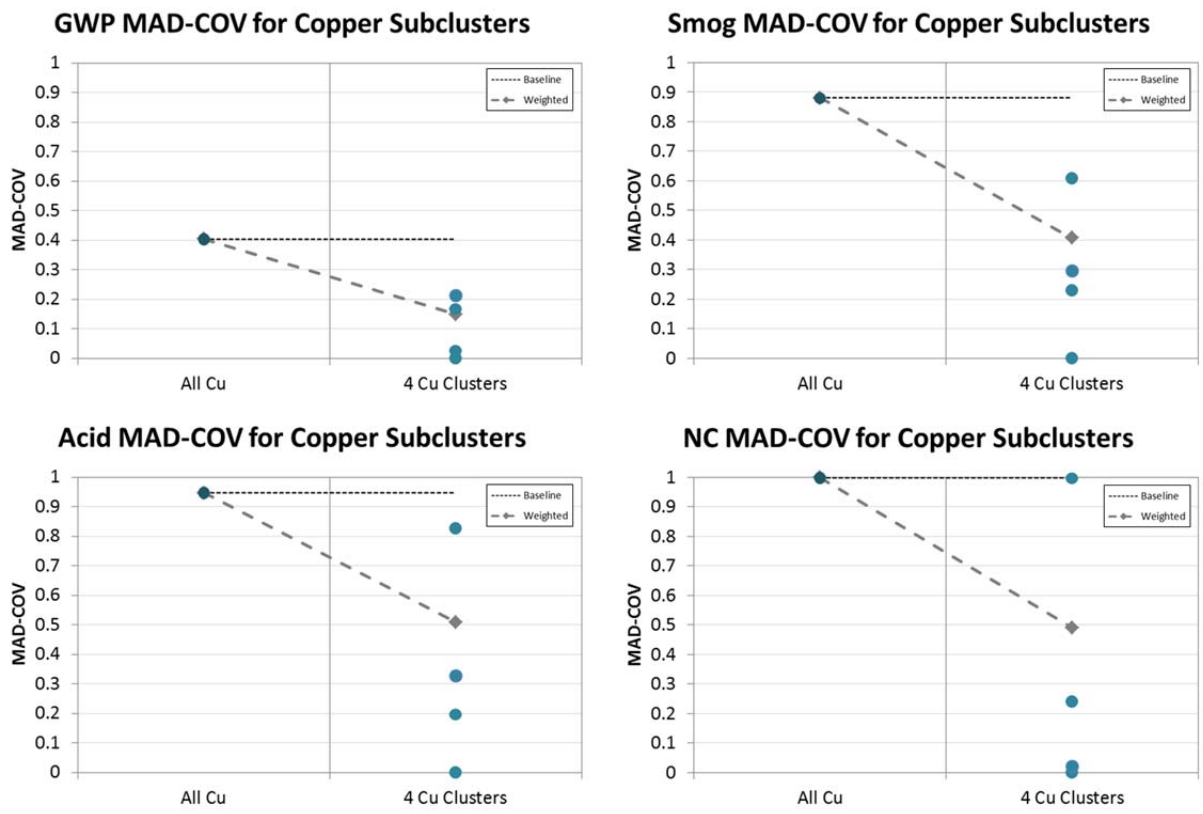

Figure 3-23. MAD-COV for all copper processes together and then after splitting into four clusters. The black dotted line shows the baseline for all copper processes together and the grey line with diamonds shows the weighted average values.

Thus, for this example of subdividing a level 3 cluster, we see that we could achieve improvements in all metrics with additional information. However, it is likely that this information goes beyond the realm of materials characteristics and into characteristics based on process information or data source. While it is intuitive that processing (as well as data assumptions) will have an influence on the environmental impacts reported, the cost of this information is assumed to be much higher than that for materials characteristics. While materials characteristics may be related to the design or assembly of a product, many processing avenues can result in the same final product. Thus, this information may represent less knowable information, and indicates that going beyond level 3 may add cost to the analysis. Considering, the combination of knowability and value in terms of increased effectiveness of the structure, these results indicate that level 2 may be a potential stopping point for our analysis.

3.2 Polymers Taxonomies

3.2.1 Dataset Formation

There were many challenges with the polymers dataset formation. Much of the data were derived from PlasticsEurope and have been re-evaluated within other databases. However, the evaluated values for environmental impacts differ across the databases, even when assessed within the same software program. Furthermore, there was not always transparency about how the data was used or adapted. Many duplicates were removed from the dataset, but some remained due to discrepancies in the end result, and it is hypothesized that others exist where it was unknown that the data originated from the same source. Due to these factors, data source is a bigger challenge within the polymers dataset than the metals, and this will be demonstrated in the results.

The scope of what is included in the polymers section is greater than in the previous work by this research group (Patanavanich 2011). A few additional bio-based materials were included as well as some other polymers not classified within the polymers groups in the software programs. In the end, 142 database entries for polymers were evaluated within this analysis. One challenge with the polymers is that they tend to have vague descriptions in the documentation. Thus, it can sometimes be difficult to determine when a material is an oligomer versus a polymer.

A number of classifiers were evaluated for the polymers. A summary is provided in Table 3-7.

Table 3-7. Classifiers evaluated for the polymers dataset

Classifier Category	Classifier
Characteristics of individual process datasets	Database source Recycled content Level of processing
Qualitative categorization of materials	Polymer type Polymer family Structural grouping Polymerization mechanism Toxicity of precursors Function
Materials properties	Price Density Tensile strength Maximum service temperature Molecular composition of base structure

As with the metals, the characteristics of individual processes were derived from the documentation. Very few recycled materials were present within the dataset as a whole. For the processing classifier, polymers ranged from precursor to polymers to semi-finished products. This grouping was based on descriptions from PlasticsEurope. The polymer family also came predominantly from a categorization developed by PlasticsEurope, with some additions required for materials they had not modeled (PlasticsEurope 2013).

Many qualitative classifications are available to describe polymers (Ebewele 2000; Eyerer 2010). The baseline grouping for previous work was based on polymer type. This included elastomer, fluoropolymer, resin, thermoplastic, and thermoset (Rampuria 2012). Some modifications were made to the baseline categorization to ensure consistency. Alternatively, the structural classification included categories similar to the polymer type, but broke thermoplastics into amorphous and semicrystalline and included soluble polymers and not fluoropolymers or resins. This categorization is slightly problematic to assess, as certain polymers can be both amorphous and semicrystalline and documentation does not always provide sufficient information to group them.

A chemist was consulted to help assign polymer processes to groups for a few of the classifiers. In the first, the polymerization mechanism was explored, and the groups were described as addition reaction or natural polymers, condensation reaction, ring opening reaction, or recycled materials. In the second, toxicity was evaluated as a separate classifier, since human health non carcinogenicity was one of the impacts under consideration. The grouping only consisted of chemicals with known toxic precursors (e.g., vinyl chloride or formaldehyde) and all other materials. This categorization was very problematic, as documentation often listed multiple reaction pathways, and precursors and catalysts were not well reported. Thus, this is a category that could be expanded upon in the future, and processes could potentially be assigned to groups based on fundamental properties as well.

The last qualitative grouping was function. According to Ullmann's Encyclopedia of Industrial Chemistry, polymers are typically grouped into four categories: commodity, engineering, high-performance, and functional. In these descriptions, commodity polymers are produced in large volume and used in many bulk applications. They may be low cost and have poorer mechanical properties. Engineering polymers typically have improved mechanical and thermal properties. High-performance polymers have even better properties, and lastly functional polymers are used in specialized applications (Elias 2000). For the purposes of this assessment, high-performance and functional polymers have been combined. A

number of resources were searched to categorize the polymers appropriately (Lesko 2008; Ebewele 2000; National Research Council 2001; The International Association of Plastics Distributors). The distinctions between groups are somewhat unclear, such as between commodity and engineering polymers. For instance, acrylonitrile-butadiene-styrene was found in both groups in different sources. One version of this structure can be seen in Figure 3-24. Although, this depiction does not exactly match what was used for analysis, it provides an idea of general properties for the function categories. Thermoset and elastomeric materials were given their own groups within the function classification and were not considered within the framework shown, although some of the literature suggested that they could be. The function categorization will obviously have overlap with categorizations based on other properties, since it is an aggregation of thermal properties, mechanical properties, price, etc.

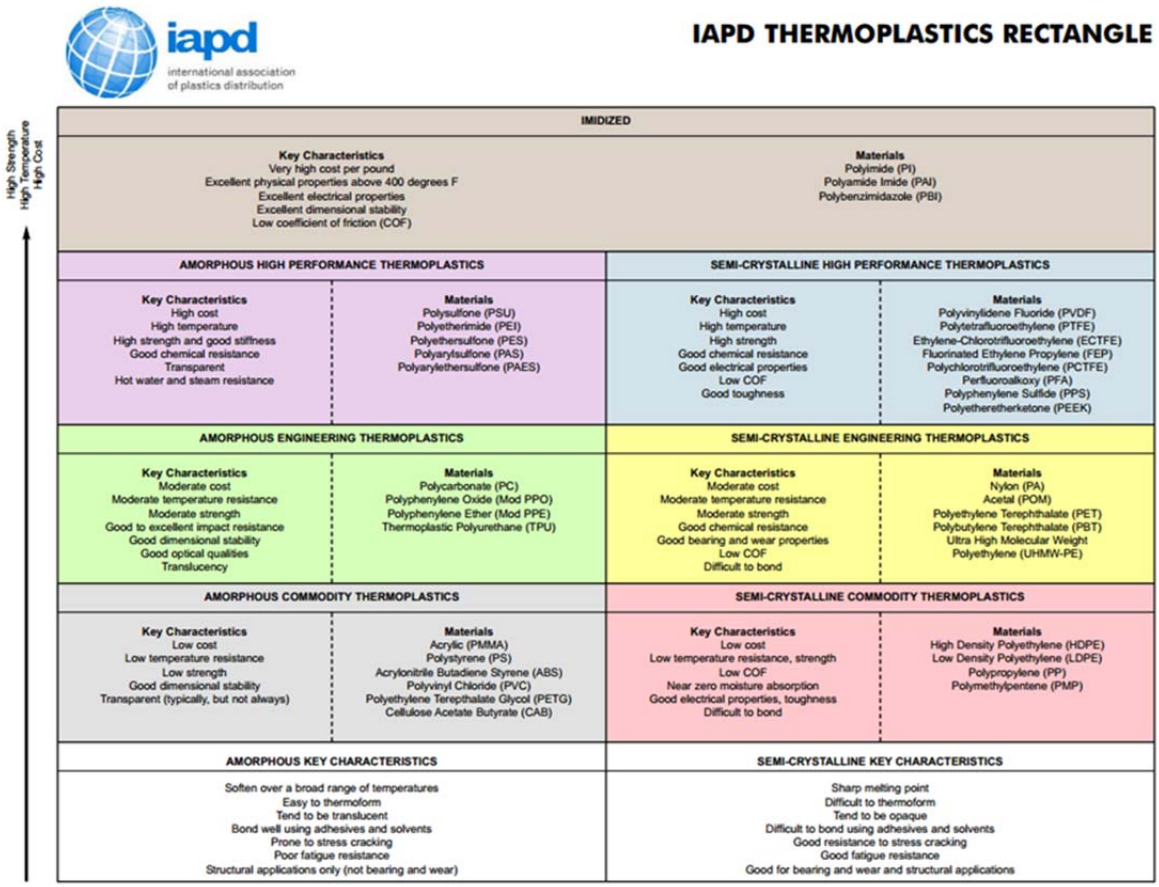

Figure 3-24. International Association of Plastics Distribution grouping of thermoplastic polymers by function. Reproduced from (The International Association of Plastics Distributors)

For material properties, price was again considered. Fewer prices were in the CES database for polymers, so some additional sources were used to determine prices, as well as a few other properties

(DuPont 2013; Omni Tech International 2010; Recycle.net 2007b; Fiebach and Grimm 2000; PPG 2007; Ebnesajjad 2013; Matweb; DuPont 2011; Demilec LLC 2013; Hercules 1999). Some of the data sources for price should be evaluated more extensively in future work, but for purposes of this analysis provided at least rough estimates of values. The maximum service temperature was considered, since this property could potentially be related to increased energy for processing. Furthermore, the molecular composition of the repeat unit was evaluated. This classifier was problematic particularly for some of the thermoset materials with varied structures, and so was not used extensively except in the consideration of certain elements (i.e., fluorine). Ideally, molecular weight would have been considered, but this information was not available in the documentation and represents a gap in the data collection.

The same four environmental impacts (acidification, global warming potential, human health non carcinogenicity, and smog formation) were used as with the metals dataset. However, it is known that the data source played a larger role within the polymers dataset for some of the impacts selected, such as global warming potential, and this was seen via regression tree analysis. Figure 3-25 shows that when the principal component scores plot is examined and colored by data source, there is some clustering of the information by source, particularly for the data from ELCD. We were not able to eliminate this source of error, leaving some error unaccounted for in the end taxonomy.

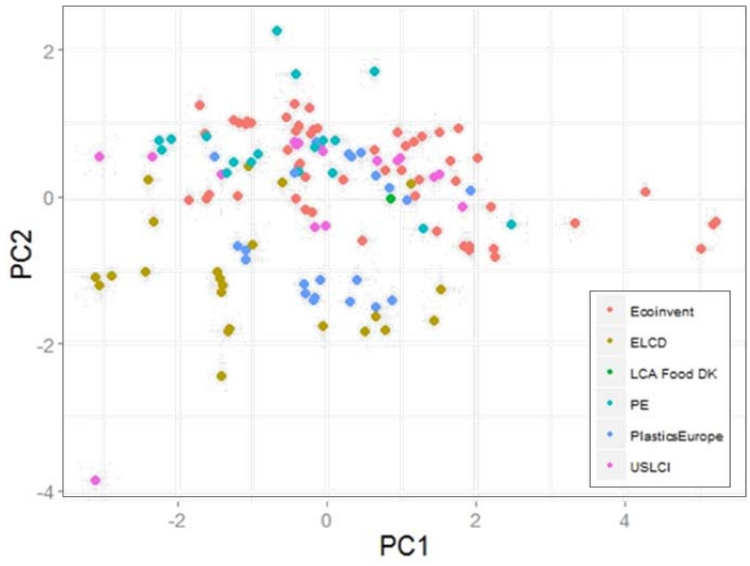

Figure 3-25. PCA scores plot colored by database source of the polymer

3.2.2 Exploratory Analysis and Classifier Identification

Data was visualized via boxplots, and Figure 3-26 highlights the presence of a very skewed distribution, with more pronounced outliers than in the metals dataset. These are confirmed with a Mahalanobis distance test. If these points were removed, most of the variability lies within the human health non carcinogenicity impact.

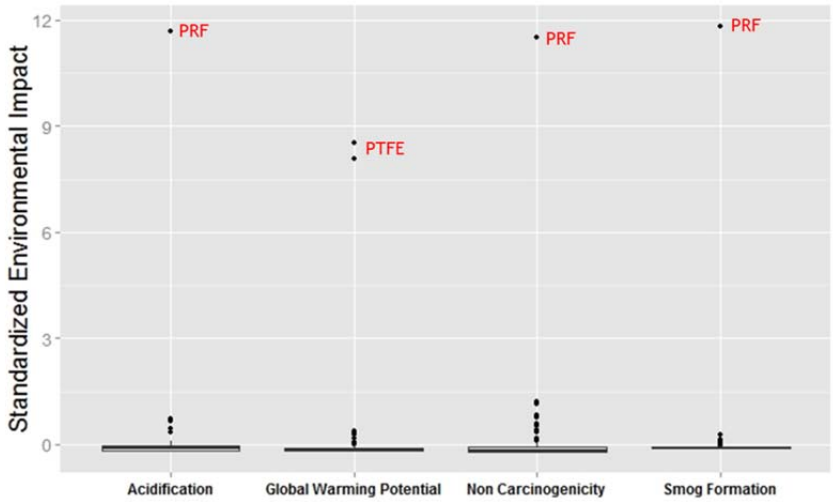

Figure 3-26. Boxplot of standardized environmental impacts for polymers with some outliers identified. Materials identified include: PRF = phenol-resorcinol-formaldehyde resin; and PTFE = polytetrafluoroethylene.

Next PCA was performed, once again showing the same significant outliers. In Figure 3-27a, we can see that in terms of the variability, all of the other data are similar when the outliers are included. Thus, we re-assess the PCA with these three points removed and find an interesting pattern in the data in Figure 3-27b. Here we see that, as with metals, the non carcinogenicity is perpendicular to the other three impacts. Unlike the metals however, we see an L-shaped pattern in the data showing one group predominantly influenced by the non carcinogenicity variation, and the other influenced by the other three impacts. This implies that some type of toxicity classifier may be useful to explore to account for this variation in the data.

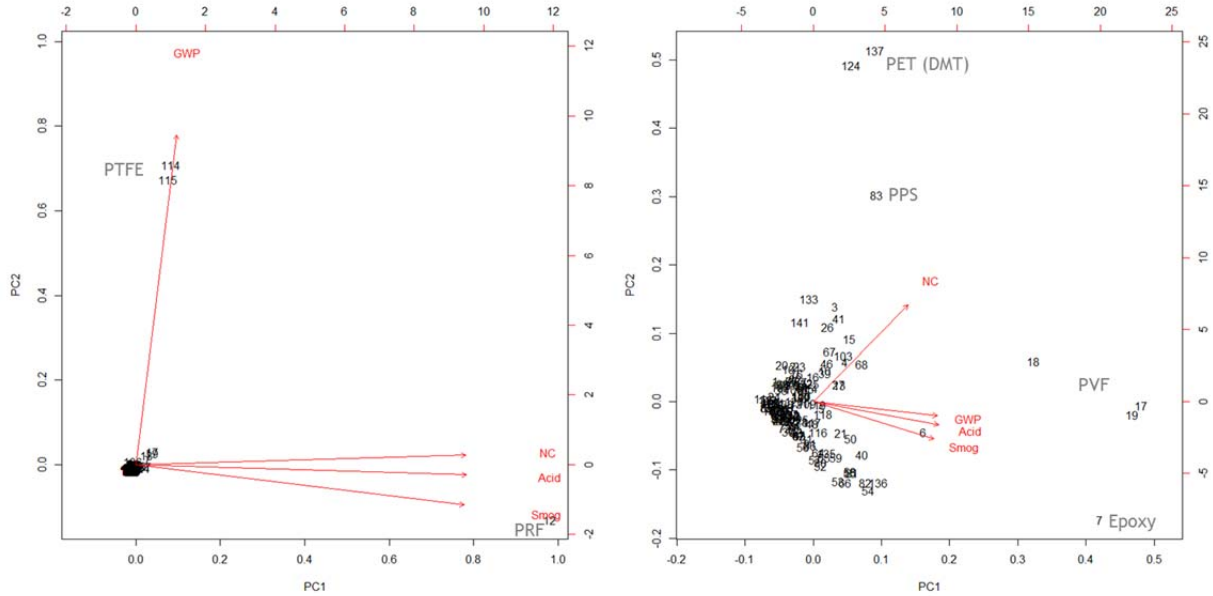

Figure 3-27. Principal component analysis on the polymers dataset with influential points indicated. Plot shows principal component 1 versus principal component 2 for all data points (left) and with outliers removed (right). Material identified include: PET (DMT) = polyethylene terephthalate produced with dimethyl terephthalate; PPS = polyphenylene sulfide; and PVF = polyvinylfluoride.

Clustering was performed using the Ward method. The knee of the joining distance scree plot showed 12 clusters, but the greatest gains were made after only four clusters were formed. Thus, this set of four clusters were explored in the first tier analysis. The environmental profiles for the clusters are shown in Figure 3-28, and descriptions of the clusters are in Table 3-8. Both outlier groups were segregated in the clustering as expected, and two additional groups were also formed. Cluster 1 contained all of the material processes that were lower in impact, and in fact barely showed up on the environmental profile compared to the other processes. Cluster 2 represented the influential points highlighted in the PCA analysis in Figure 3-27b. Interestingly, this cluster contained both polymers significant in non carcinogenicity as well as ones with high values for the other impacts. It was somewhat difficult to describe this group, but in general it contained higher temperature and higher cost polymers. The PET was difficult to explain, since PET from similar production pathways was found in the rest of the data, and this did not seem to fit intuitively with the rest of cluster 2.

Table 3-8. Summary of polymers clusters at level 2. Specific database entries include: LDPE = low density polyethylene; PMMA = polymethylmethacrylate; PVC = polyvinylchloride; and SBR = styrene-butadiene rubber.

Cluster #	Cluster Name	Cluster Description	Example Database Entries
1	Most polymers	Lower impact polymers – may include elastomers, commodity, and engineering polymers	LDPE PMMA PVC SBR
2	High Temperature Polymers? Specialty?	Polymers influential in any impact	Epoxy PET (DMT) PPS PVF
3	PTFE	PTFE	PTFE film
4	PRF	Only includes one material	PRF resin

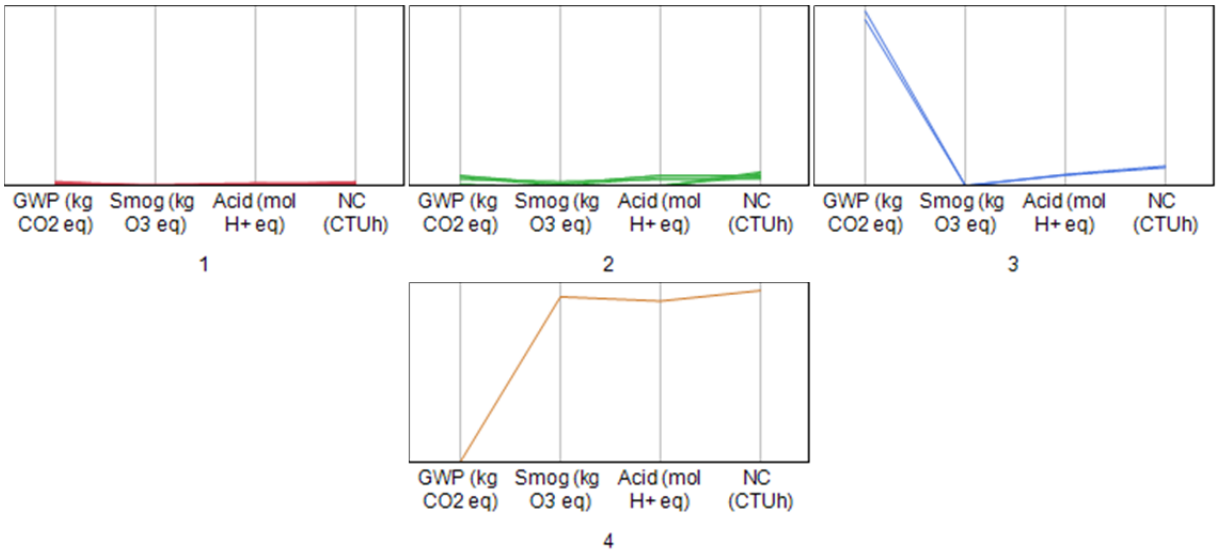

Figure 3-28. Environmental impacts of polymers in each cluster by cluster number

Due to known data source problems within the polymers dataset, clustering analysis was also performed on each data source individually. This analysis highlighted that the function of the polymers seemed to explain the clusters. Although, higher performance polymers were not present in every data source, segregation of commodity and engineering polymers was evident.

A few classifiers were significant from the exploratory analysis. These included price, maximum service temperature, function, and toxicity. Function and price were both also identified in the metals dataset; however temperature and toxicity are specific to the polymers data. Both price and maximum service temperature are examined by cluster in Figure 3-29. In both cases, the properties are fairly distinct by

cluster for the bulk of the materials, but there is some overlap in the tails. In terms of function, all commodity and elastomeric polymers are present in cluster 1, although the engineering polymers appear in multiple clusters. All analyses highlighted the same outliers, so these were once again segregated into their own groups. Other phenolic and formaldehyde based resins are present in the dataset, but do not show the same influence as the PRF point highlighted. Although the other database entries are not exactly the same material, they indicate that the PRF database entry should be further explored.

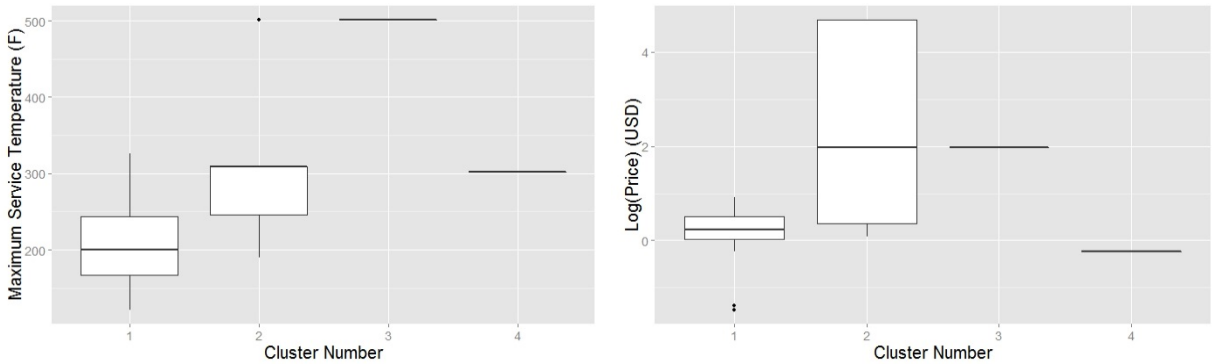

Figure 3-29. Maximum service temperature by cluster number for polymers data (left) and price by cluster number (right)

3.2.3 Classifier Evaluation

PCA showed that the logarithm of the price was most highly correlated with the first PC (r=-0.56), which was less than in the metals data set. Maximum service temperature (r=-0.50) and percent fluorine within the repeat unit (-0.53) had only slightly lower correlations. While price did appear to have some trend outside of outliers, the other two parameters seemed to be valuable mostly for discriminating only the highest points. The boxplots of categorical classifiers showed less clear distinction than in the case of the metals. The polymerization category was one of the best, with recycled polymers much lower than other categories and some distinction between addition, condensation, and ring opening polymers. Function categories showed some trending as properties improved, but again overlap was seen, especially for thermoset polymers, which were not considered within the properties framework. The distinction between commodity/elastomer and engineering/functional/thermoset polymers became clearer if the polymers with toxic precursors were eliminated, but the polymers with toxic precursors had similar values of PC1 to other groups. Data source showed the most distinction with PC2, mostly for data from ELCD.

In terms of the SSW/SST metric, many categorizations were similarly able to reduce the uncertainty across impacts by approximately 40-45%. Thus, there is likely to be some overlap in the variation that they capture (i.e., between price, function, and maximum service temperature). The one that reduced uncertainty the most was data source, indicating that data source was still a problem within this data. For all categorizations, the worst performance was for non carcinogenicity, even for the toxicity classifier, which did not outperform others for that impact.

The logistic regression models did not perform very well for this dataset. The best models had a 5-25% misclassification rate for the training data, but low improvement rates. The best improvement rate in training data was seen with the data source, which had a 78% improvement rate. However, this dropped in the validation data. The categorization segregating polymers with high maximum service temperatures had a very low misclassification rate, which was maintained in the validation data, but showed 0% improvement on validation data given that the baseline was quite high. For price, polymerization, and polymer type, the misclassification rate did not drop significantly between training and validation data, but the improvement levels were too low to suggest a good predictive model. Toxicity showed some improvement on validation data, although it had about a 40% misclassification rate. Thus, only data source was really promising for this metric, although price and toxicity also showed some improvement.

Linear regression was performed with the three outliers removed, since they were very evident in the residuals patterns. With those removed, a reasonable R^2 of 0.77 was achieved. Two database sources were significant in the prediction as were the price and the function categories. Even though functions were not all individually significant, as a group they passed the partial F test. Lastly, whether the polymerization method was ring opening or not was a significant variable. If this parameter was omitted, the model still performed fairly similarly, but it was included due to the significant p-value. There was a little multicollinearity, but well below any levels for concern, and residuals approximated normality nicely.

The regression tree algorithm first separated the previously identified outliers. Thus, further analysis was performed with the outliers removed. After removal, the first division segregated high temperature polymers. The next split was made based on the price of the materials. Residual variation was captured to a lesser degree by the data source and polymerization mechanism. Although the k-fold R^2 was only 0.50, it was fairly close to the overall value. A simplified, pruned tree can be seen in Figure 3-30.

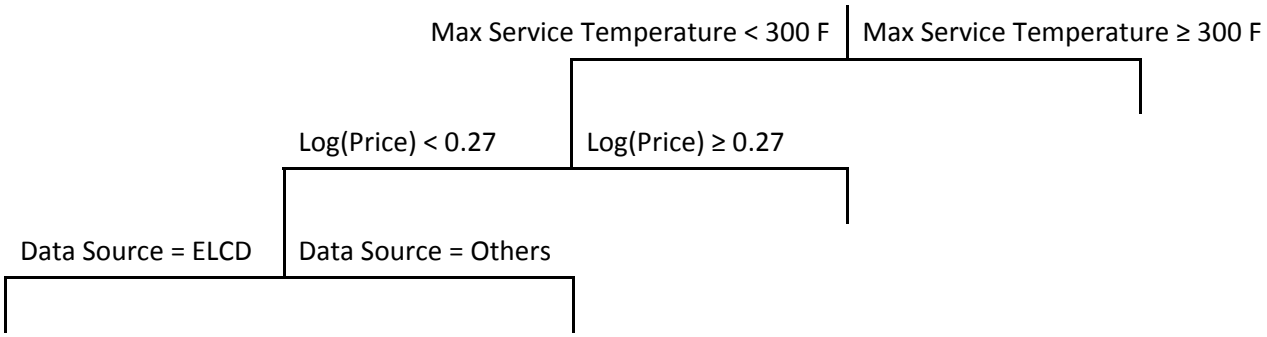

Figure 3-30. Regression tree for polymers with outliers removed showing splits based on maximum service temperature, price, and data source

The summary of all of the classifier evaluations is shown in Table 3-9. Unlike for the metals, there was no clear winner. Price and data source were the most dominant classifiers, but once again data source is of little interest from an applications perspective. Other potentially important classifiers were maximum service temperature and polymerization mechanism. One explanation for why so many parameters appeared significant in these evaluations is that none of the classifiers were fully capturing the variation within the data, and that a better categorization could potentially exist. Alternatively, there may be some overlap between the ways these classifiers group the materials. A final explanation is that the variation in the impacts for polymers may be relatively small, leading to many possible classifiers. Lastly, it is interesting to note that once again the baseline (polymer type) showed very little significance. Thus, this implies that this method can improve on qualitative classification methods.

Table 3-9. Summary of classifier evaluation for the polymers

	Polymer Type	Data Source	% Fluorine	Price	Max Service Temp	Function	Toxicity	Polymer-ization
PCA			x	x	x			
SSW/SST		x		x	x	x	x	x
Logistic Regression		x						
Linear Regression		x		x		x		x
Regression Trees		x		x	x			x

3.2.4 Taxonomy Formation

As no classifier stood out as exceptional in the previous analyses, the entire set of classifiers was considered for effectiveness and efficiency. The seven types of structures evaluated are shown in Table 3-10. The threshold values for continuous classifiers were selected from the regression tree analysis or from threshold value examinations using effectiveness metrics. In addition to the groups listed in the table, all categorizations contained a group for the single PRF database entry and a group for the two PTFE ones.

Table 3-10.Summary of polymers level 2 proposed taxonomies

Baseline	Data Source	Function	Polymerization	Max Service Temp (F)	Toxicity Combo	Price ($/lb.)
Type	DS	Func	Poly	MST	Tox	Price
Elastomer Fluoropolymer Resin Thermoplastic Thermoset	Ecoinvent ELCD LCA Food DK PE PlasticsEurope USLCI	Commodity Elastomer Engineering Functional Thermoset	Addition/Natural Condensation Recycled Ring Opening	A: <300 B: ≥300	MST-B (>300) Toxic Precursor Comm/Elast[5] Other	A: ≤ 1.45 B: 1.45<P≤5 C: > 5

The level 1 MEDAPEs for the polymers were lower than those seen in the metals dataset, particularly for smog and acidification. The proposed level 2 taxonomies were all able to slightly reduce the MEDAPE as shown in Figure 3-31. Although data source performed best overall, the difference was not large, and all of the taxonomies showed fairly similar performance. The reduction from level 1 to level 2 was much less than for the metals. Data source, the best performer, reduced the average MEDAPE from 55% at level 1 to 43%. Although the average MEDAPE at level 2 was comparable to that for metals, the improvement was less significant. Once again, the highest error rate was seen for non carcinogenicity, and in this dataset the other three impacts had fairly comparable error rates.

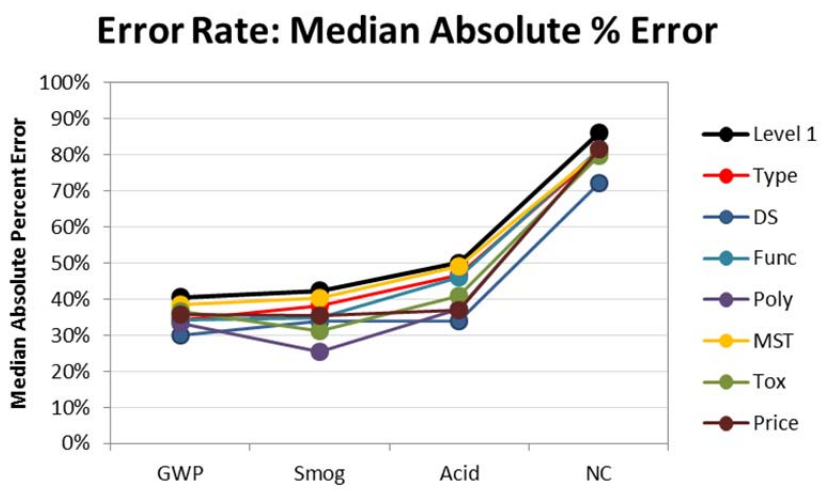

Figure 3-31. MEDAPE for level 1 polymers and level 2 polymers proposed taxonomies

For the percentage of materials that improved based on a given structure, the results were again fairly comparable across proposed taxonomies as seen in Figure 3-32. Thus, the error rate for all was reduced

[5] Commodity/Elastomer

for approximately the same number of materials and by the same magnitude. The improvements were even smaller than with the metals, suggesting that the intermediate levels proposed for the polymers structure provide less value.

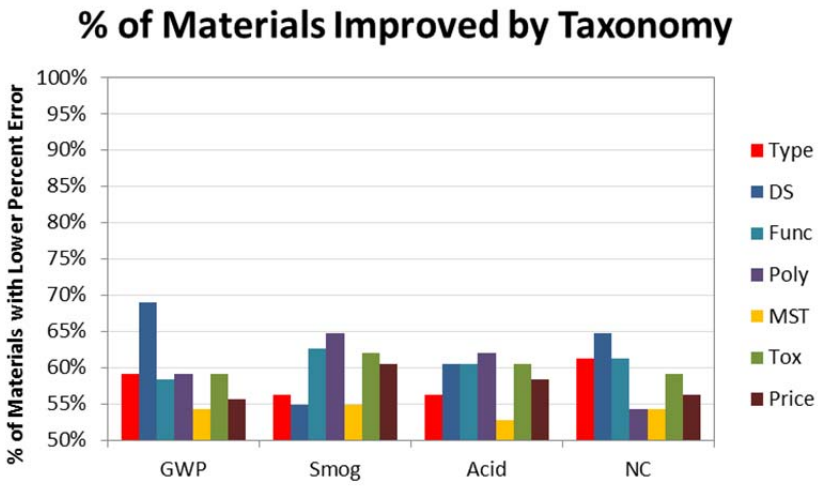

Figure 3-32. Percent of polymers for which the percent error was less in level 2 proposed taxonomies

The outliers accounted for the majority of the uncertainty in the dataset. With the outliers in their own groups within the structure, all taxonomies showed a residual SSW/SST of 0-3% for all impacts. Thus, in order to get a realistic assessment, the outliers were removed from the calculation of the total sum of squares to obtain the plot in Figure 3-33. Here polymer type (baseline) and price were the best at accommodating the outliers in the data, whereas data source and polymerization method were the worst.

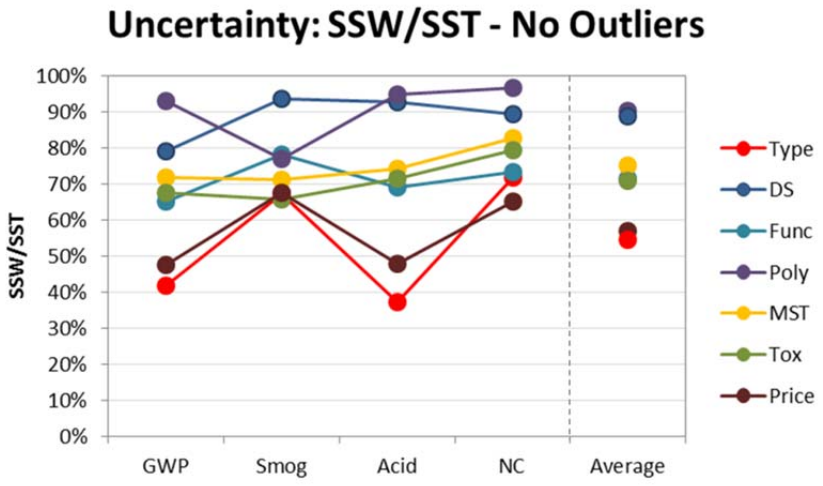

Figure 3-33. SSW/SST for level 2 polymers proposed taxonomies

The uncertainty for the groups is shown in Figure 3-34. There was some improvement by grouping the polymers into taxonomies, although less so than in the case of the metals. The level 1 MAD-COVs were much lower than with the metals, except in the case of non carcinogenicity. Data source showed the most improvement across taxonomies, except in smog formation. After that, price seemed to perform the best overall with more groups that were below the level 1 baseline and with lower weighted values. Once again however, there was a lot of similarity across structures.

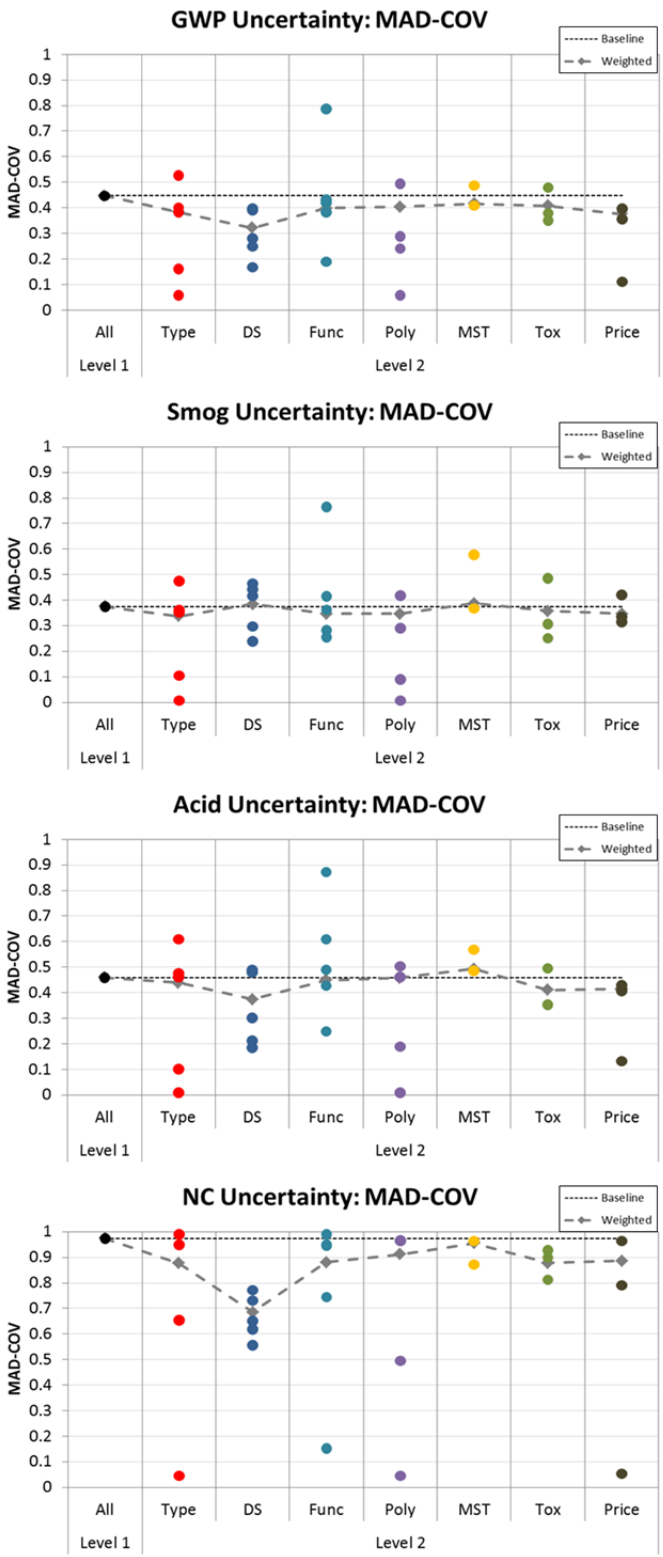

Figure 3-34. MAD-COV values by group within each proposed level 2 polymers taxonomy. The black dashed line represents the baseline value set by level 1. The grey diamonds show the weighted average MAD-COV for each proposed taxonomy. Groups with a single element and a MAD-COV of zero have been removed.

In terms of efficiency, proposed classifications differed in the number of groups more than for metals as shown in Table 3-11. Price and maximum service temperature had relatively fewer, while the type, data source, and function had relatively more. In absolute terms, the difference is not great, but we did see differences in the efficiency of distinguishing between the groups in a given taxonomy, as shown by the distinction rate in Figure 3-35. The polymer type had relatively poor efficiency while the price, maximum service temperature, and polymerization mechanism had very high efficiency.

Table 3-11. Number of groups in each level 2 polymers proposed taxonomy

	Type	DS	Func	Poly	MST	Tox	Price
Number of Groups	7	8	7	6	4	6	5

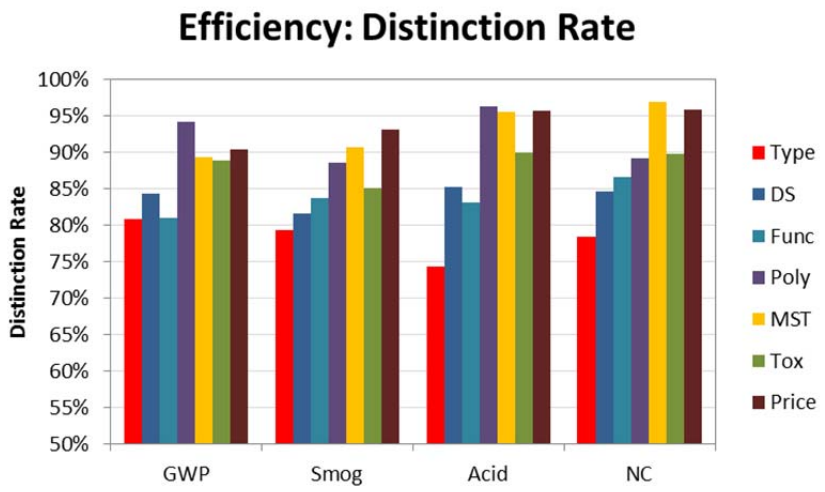

Figure 3-35. Distinction rate for level 2 polymers proposed taxonomies

The lower efficiency for type, data source, and function were all seen in the overlap between the categories when compared to the PCs. For instance, classification by data source may only require the segregation of the ELCD group for effectiveness, and thus the additional groups would only reduce efficiency. Function might be able to be improved if the performance criteria could be extended to the thermoset and elastomer groups, which at this time had significant overlap with other categories.

Toxicity performed fairly well, but additional documentation and evaluation of other properties could potentially improve this group. It likely has potential to reduce the large variation seen in the non carcinogenicity category if more distinct groups could be created or the PET compounds could be

explained. Some decrease was seen in the MAD-COV for non carcinogenicity, but it is expected that this could be further improved.

Price and maximum service temperature had the highest efficiencies, but price performed better on the effectiveness criteria. Price also had improved effectiveness ratings over the polymer type (previous structure), while demonstrating a higher efficiency. Thus, price was selected as the best taxonomy for further analysis. This is also consistent with the metals analysis, and price is a knowable characteristic.

3.2.5 Next Tier Analysis

Subsequent cluster analysis on the price taxonomy showed some additional challenges in the data. The high price group was too small to cluster, but accounted for a large percentage of the residual uncertainty, and so material types were simply split out. For the low-priced group, no intuitive categorization apart from data source was evident in examining the clusters. Thus, the low price group was left as a single entity. Within the medium-priced category, it was also difficult to discern patterns in the data. However, of the five clusters evident in the medium-priced category, a few things stood out. For one, two of the clusters were predominantly nylon based materials (nylon 6 and nylon 66, filled and unfilled). The only thing segregating the two different nylon clusters was again the data source. Therefore, for the proposed taxonomy, all nylon compounds were grouped together. One epoxy database entry also formed its own cluster, so a group was created containing all epoxy materials as well. This produced the three level hierarchy shown in Figure 3-36. This structure only had eight groups, similar to some of the proposed level 2 taxonomies.

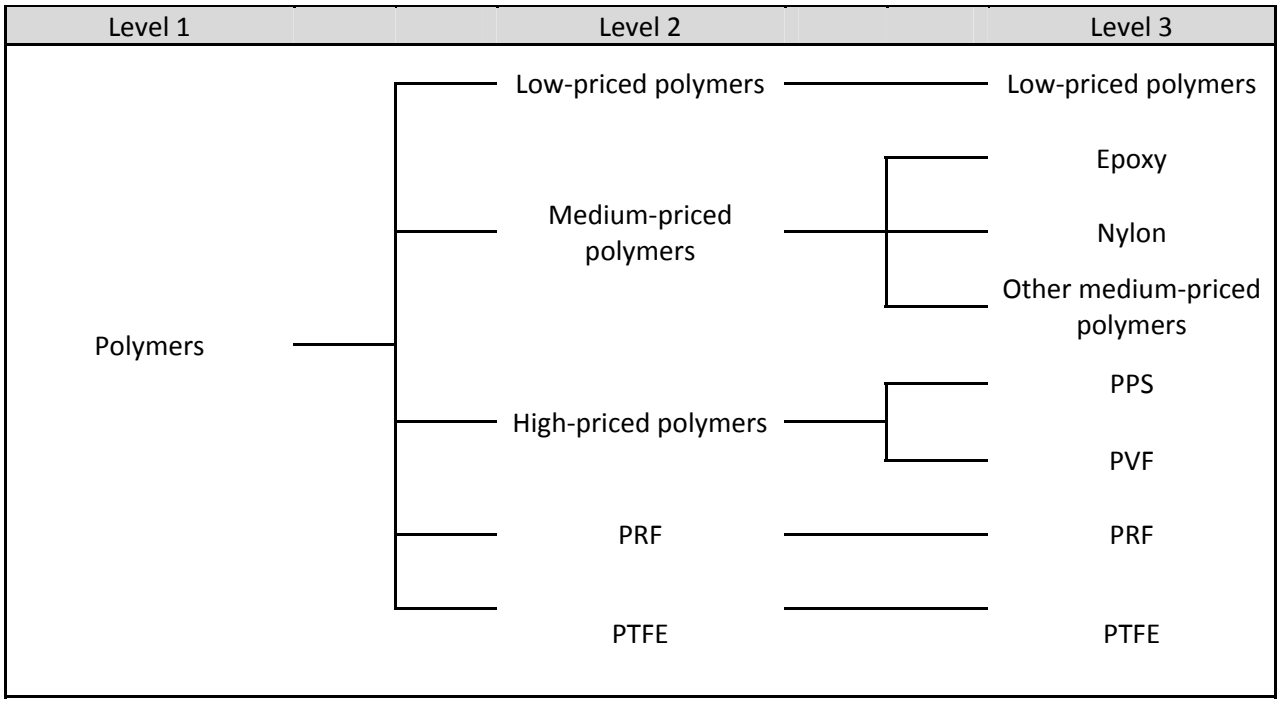

Figure 3-36. Proposed level 2 and level 3 hierarchy for polymers

The additional categories in level 3 reduced the average median absolute percent error from 47% to 44% and the SSW/SST from 67% to 60% as shown in Figure 3-37 and Figure 3-38. In terms of MAD-COV, there was a marginal decline in the weighted value, but a few groups with higher MAD-COV, illustrated in Figure 3-39. Those were the epoxy group for global warming potential and the PVF group for smog formation. This effect for the epoxy group was expected, since the one epoxy database entry could not be differentiated appropriately. Despite these improvements in effectiveness, the level 3 structure was only an improvement for 18-23% of materials over level 2. Thus, the level 2 structure had a lower absolute percent error for many more of the materials, despite higher absolute improvement for a few. Furthermore, the distinction rate was 83-89%, which was a drop from what it was at level 2. Therefore, it appears that the level 3 structure for polymers did not add a lot of value.

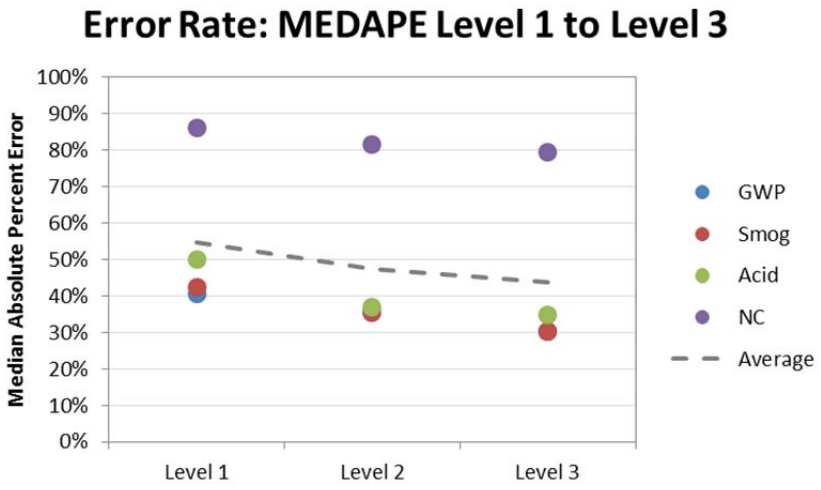

Figure 3-37. MEDAPE for polymers from level 1 to level 3

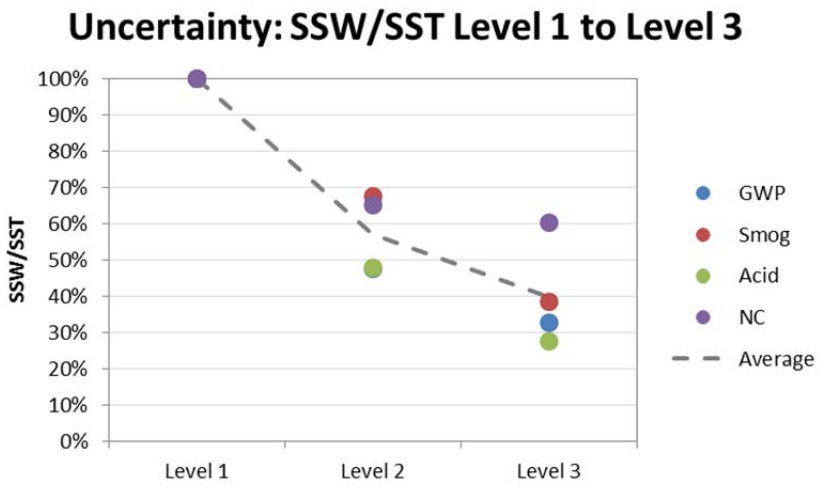

Figure 3-38. SSW/SST for polymers from level 1 to level 3

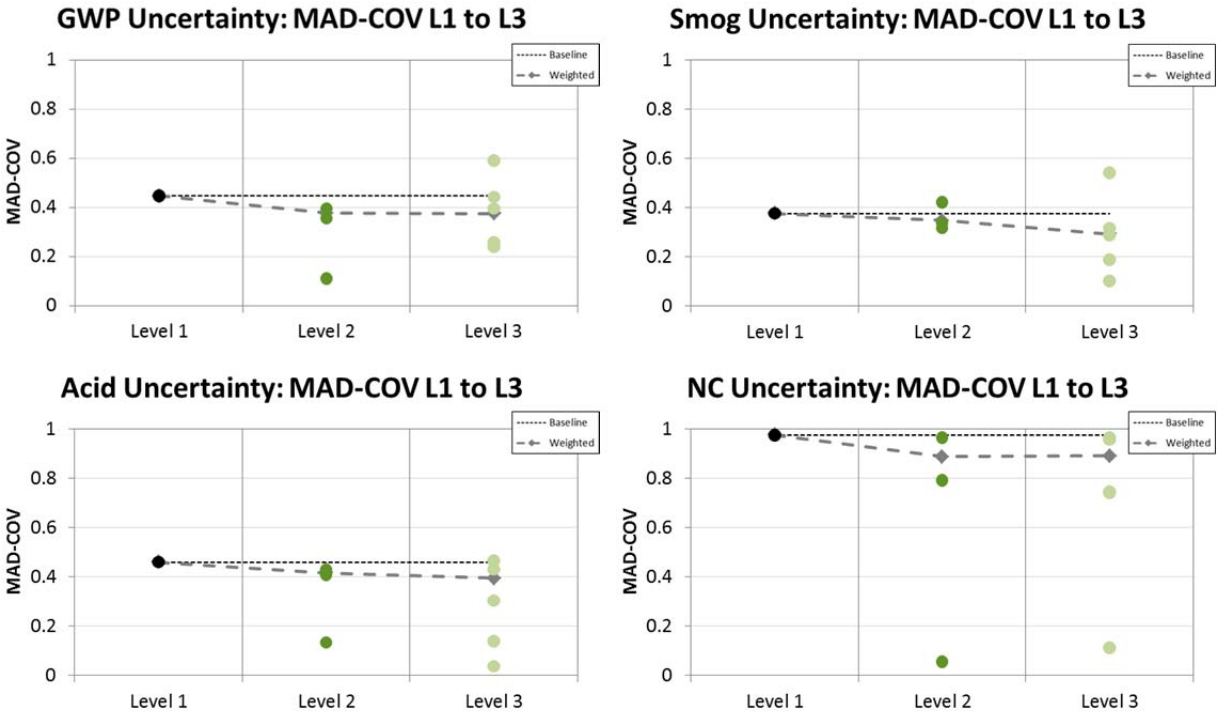

Figure 3-39. MAD-COV from level 1 to level 3 for price and then price subcategories. The black dashed line represents the baseline value set by level 1. The grey diamonds show the weighted average MAD-COV for each proposed taxonomy. Groups with only one element and a MAD-COV of zero have been removed.

3.3 Precious Metals Taxonomies

3.3.1 Dataset Formation

The precious metals dataset was chosen as a final example, since it was a small dataset made up of only materials from a single data source. Other precious metals data exists, but we did not have access to it for this study. The dataset consisted of only 36 database entries, which is small for some of the methods applied in previous categories, but the increased consistency made it easier to draw conclusions. A list of the classifiers evaluated is shown in Table 3-12. This was more limited than the previous materials categories because of greater similarities in the materials (only five different metals are included).

Table 3-12. Classifiers evaluated for the precious metals dataset

Classifier Category	Classifier
Characteristics of individual process datasets	Recycled content Location
Qualitative categorization of materials	Material type
Materials properties	Price

Recycled content and location of the mine were based on the descriptions in the documentation. Some database entries were an aggregation of materials from different mines, and for those the location listed for the database entry was considered. The material type was easy to determine, and as mentioned five types were included (gold, palladium, platinum, rhodium, and silver).

Lastly, price was evaluated as a classifier. Similar to other datasets, the price information was taken from the CES database, except in the case of rhodium, which was not in the database. For rhodium, the average price from the USGS from 2007 to 2011 was used (U.S. Geological Survey 2012). For precious metals, price can be highly variable and subject to complex global dynamics. Thus, price is a difficult classifier to use within the precious metals dataset, as it can change dramatically over time. Even with volatility, the price did serve to differentiate silver from other materials, as its price differed by orders of magnitude.

3.3.2 Exploratory Analysis and Classifier Identification

Visualization of the data in Figure 3-40 shows that there are fewer outliers than in the other datasets. A few influential points were highlighted. In terms of outliers, the most extreme was rhodium from

Russia. This is the same mine that produced the high acidification nickel in the metals dataset. The high points in acidification just below the rhodium are the other platinum group metals produced from that mine as well.

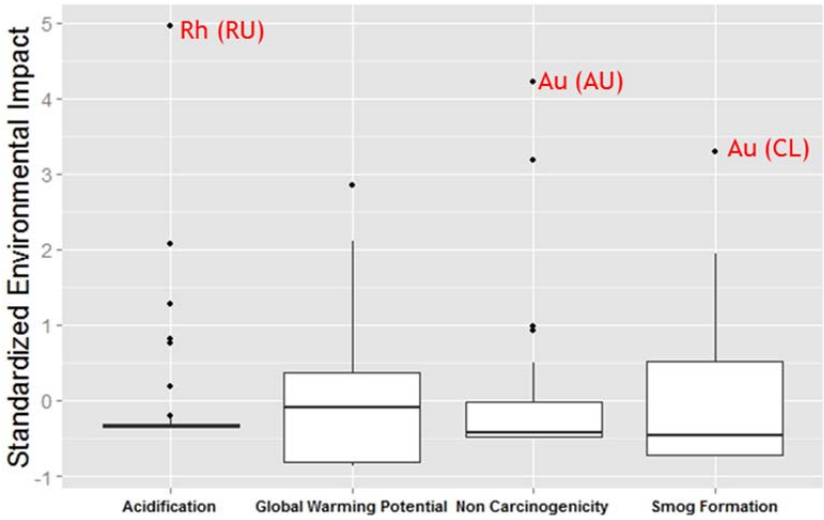

Figure 3-40. Boxplot of standardized environmental impacts for precious metals with some outliers and influential points identified. Materials identified include: Rh = Rhodium; Au (AU) = Gold from Australia; and AU (CL) = Gold from Chile.

Principal component analysis showed some interesting groupings within the data. As expected, the acidification was somewhat contrasted to other impacts due to the metals that come from the Russian mine. The contrast of impacts was also different than previous datasets, likely because of this high acidification influence. Also unlike other datasets, a line can be drawn that mostly distinguishes the platinum group metals from the gold on the plot. That line has been superimposed on the plot in Figure 3-41. The cluster of metals at the center of the figure consisted of secondary metals and the silver database entries.

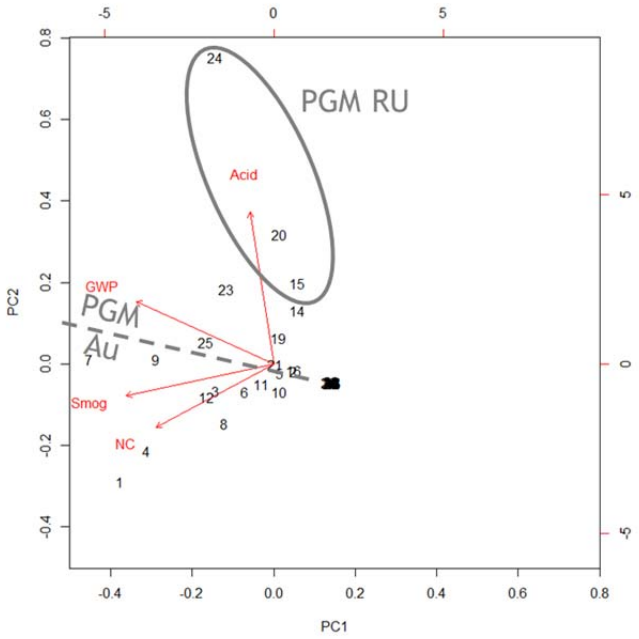

Figure 3-41. Principal component analysis on the precious metals dataset with influential points indicated. Plot shows a general divide between gold and platinum group metals. PGM stands for platinum group metals.

Lastly, clustering was performed on the dataset. The dataset was somewhat small for clustering analysis, which led to a less distinct knee in the distance joining scree plot. The environmental profiles at four clusters had a high level of variability, and so six clusters were explored here. A description of the clusters is in Table 3-13 and the environmental profiles are shown in Figure 3-42. Once again we see the secondary metals and silver grouped together in a low impact group. The rhodium from Russia formed its own cluster as well. More interestingly, we again see the segregation of gold and platinum group metals. The gold formed three separate clusters based on the location of the mines. Sufficient information about these mines was not available to discern the meta characteristics distinguishing these mines (e.g., a certain type of extraction method or different ore quality). To differentiate these processes may require the addition of similar process information as was described with copper. Thus, we can justify the exclusion of this information on the basis of cost of information. In general, the gold seemed to be higher in smog formation, and if this factor was not included, gold may not have clustered separately from the platinum group metals.

Table 3-13. Summary of precious metals clusters at level 2

Cluster #	Cluster Name	Cluster Description	Example Database Entries
1	Gold 1	Gold from AU and US	Gold from Australia Gold from United States
2	Gold 2	Gold from CL and PG	Gold Chile Gold from Papau New Guinea
3	Primary PGM	Palladium, platinum, and rhodium	Palladium from Russia Platinum from South Africa
4	Gold 3	Gold from other places	Gold from Sweden Gold from Tanzania
5	Secondary metals and silver	All of the silver and secondary gold and PGM	Silver from Sweden Secondary palladium Secondary silver
6	Rhodium from RU	Rhodium from RU	Rhodium from Russia

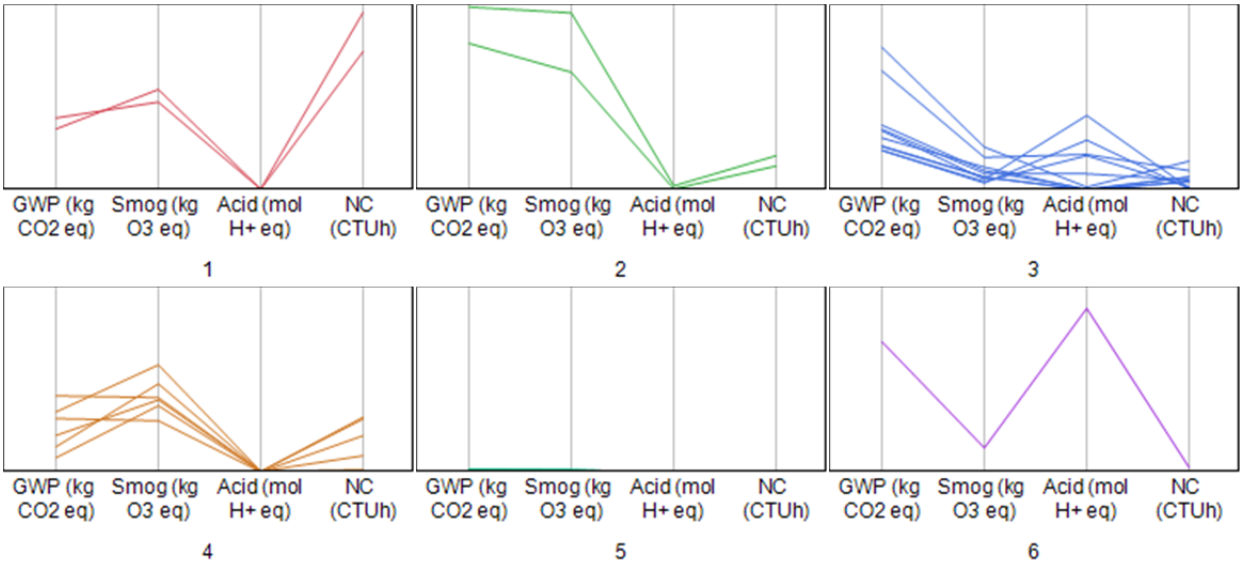

Figure 3-42. Environmental impacts of precious metals in each cluster by cluster number

From this analysis, the material type and recycled content seemed to be important classifiers. As mentioned, if more information about mining practices were available that could be useful as well. That information may be less knowable from a manufacturer's perspective, but may become more so with increasing awareness throughout the supply chain. Classifier evaluation was omitted for this dataset due to the small number of entries and classifiers involved. It was determined that the exploratory analysis was sufficient in identifying classifiers for taxonomy formation and prediction.

3.3.3 Taxonomy Formation

A few permutations of possible level 2 taxonomies are shown in Table 3-14. In general, these differed by whether or not they separated out gold from the platinum group metals and whether or not they separated out the secondary silver database entry from the primary silver.

Table 3-14. Summary of precious metals level 2 proposed taxonomies

Primary and Secondary Materials			
R1	R2	R3	R4
Ag all	Primary Ag	All Ag	Primary Ag
Primary Au/PGM	Secondary Ag	Primary Au	Secondary Ag
Secondary Au/PGM	Primary Au/PGM	Primary PGM	Primary Au
	Secondary Au/PGM	Secondary Au/PGM	Primary PGM
			Secondary Au/PGM

The level 1 MEDAPE values for precious metals were higher on average than the other datasets, particularly in acidification and smog formation. Examining the level 2 values for the proposed taxonomies in Figure 3-43, it can be seen that R3 and R4 demonstrate significant improvement in smog formation and acidification. This is due to the segregation of the gold and platinum group metals, which corresponds with the environmental profiles seen from the clustering analysis that showed gold to be differentiated by its higher impacts in smog formation. There appeared to be some lesser improvements from the segregation of the secondary silver as well (R1 to R2 and R3 to R4). The precious metals showed a similar average MEDAPE at level 2 to the other two datasets.

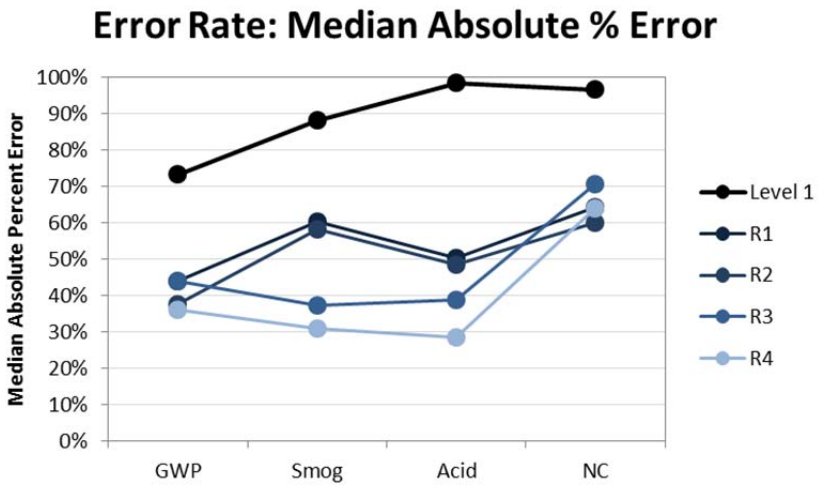

Figure 3-43. MEDAPE for level 1 precious metals and level 2 precious metals proposed taxonomies

In terms of the percentage of materials improved, similar average performance can be seen across proposed taxonomies in Figure 3-44. R1 and R2 performed better for acidification and non carcinogenicity, and R3 and R4 performed better for smog, as expected. The percentage of materials for which the structure improved the error was also much higher than for the other datasets.

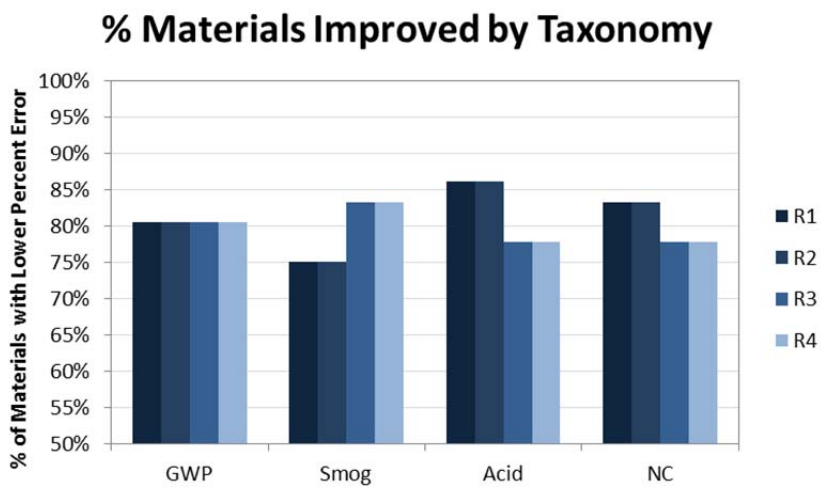

Figure 3-44. Percent of precious metals for which the percent error was less in level 2 proposed taxonomies

For the SSW/SST metric, we see in Figure 3-45 that R3 and R4 showed improvement over R1 and R2. The secondary silver accounted for very little of the overall variation in the data, causing the overlap in the chart. Based on the SSW/SST, R3 and R4 were equally good at accounting for the outliers in the data, further indicating that a segregation of gold and platinum group metals was valuable.

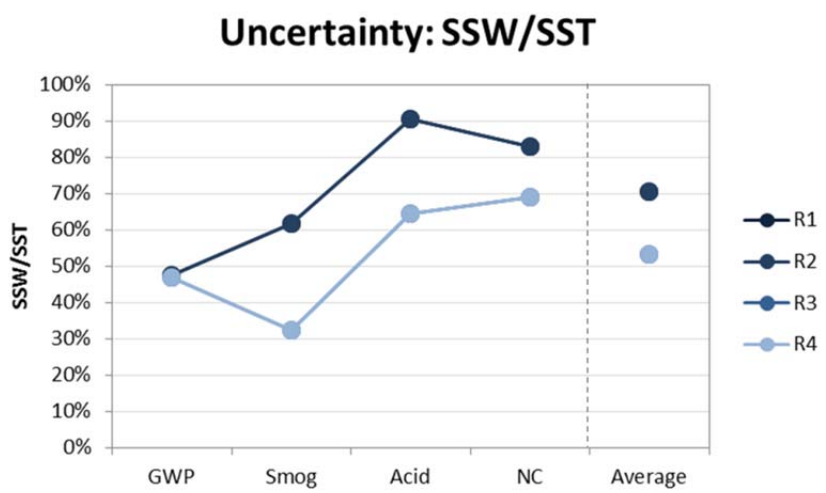

Figure 3-45. SSW/SST for level 2 precious metals proposed taxonomies

Lastly, Figure 3-46 shows the uncertainty by group through the MAD-COVs. Here all structures improved on the baseline, since the baseline started at a very high level. All groups were lower for R2 and R4 in global warming potential and smog because of the effect of the recycled silver. For acidification, the uncertainty present within the platinum group metals showed up more in R3 and R4, since the group size had diminished. Overall, R4 performed the best and showed decreases in all of the weighted values as well. Thus, there appeared to be benefits from segregating both the gold from the platinum group metals and the recycled silver from primary silver.

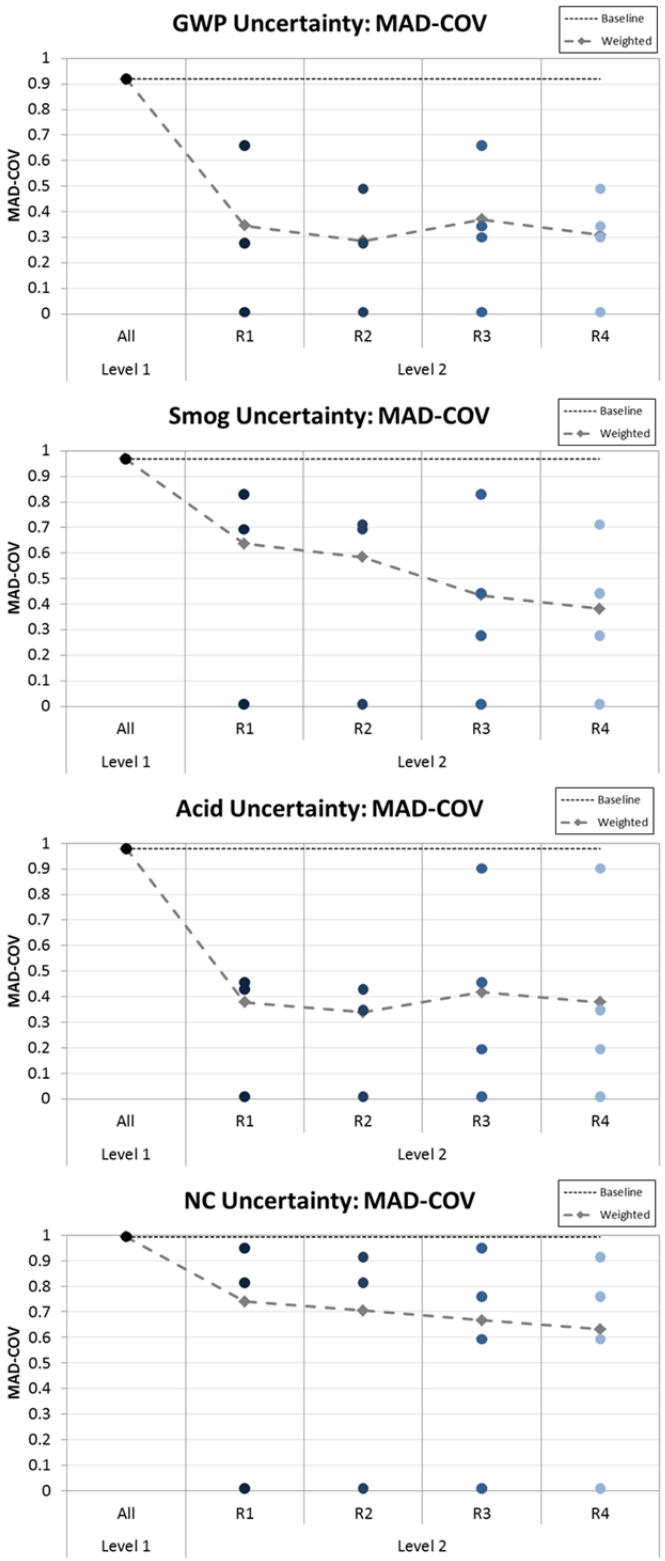

Figure 3-46. MAD-COV values by group within each proposed level 2 precious metals taxonomy. The black dashed line represents the baseline value set by level 1. The grey diamonds show the weighted average MAD-COV for each proposed taxonomy. Groups with a single element and MAD-COV of zero were removed.

In terms of efficiency, we progressively add more information from R1 to R4, shown by the number of groups in Table 3-15. The distinction rates were quite high for this dataset as can be seen in Figure 3-47. The worst overall performance was seen with R3, however even this level was higher than in prior material categories. Thus, from the perspective of being able to distinguish between groups, separating out the secondary silver added efficiency value. Thus, if the cost of this information is not too high, it should be incorporated. Overall, it seemed that R4 provided the most effectiveness and efficiency, but did have a slightly higher information cost. The proposed taxonomy for precious metals outperformed the other metals category, but this was expected due to the smaller and more consistent dataset.

Table 3-15. Number of groups in each level 2 precious metals proposed taxonomy

	R1	R2	R3	R4
Number of Groups	3	4	4	5

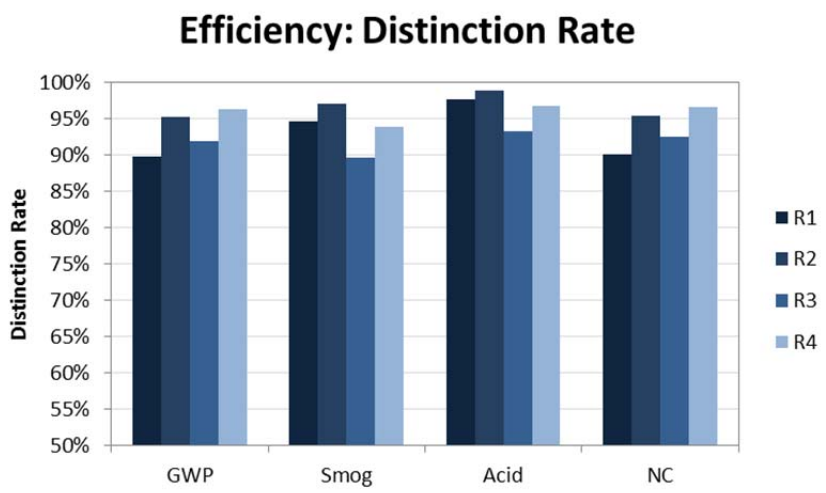

Figure 3-47. Distinction rate for level 2 precious metals proposed taxonomies

As clusters were already quite small, next tier analysis was not performed on this dataset. Any further analysis would require more specific knowledge of the mines and process information, as discussed for metals.

3.4 Summary of Materials Taxonomies

In this section, we saw that the quantitative methods were beneficial in helping to develop effective and efficient taxonomies. The structures created using the quantitative framework showed improvement over those developed in the previous work using only qualitative methods based on this set of metrics for effectiveness and efficiency. For the metals, classification based on three generic price groupings at level 2 was able to reduce overall uncertainty by 55%, while showing median error rates of 30-40% for all impacts except non carcinogenicity. This is compared to initial median error rates of 59-94% for these impacts. Furthermore, the average distinction rate of 91% indicated a fairly high ability to differentiate between groups to enable decision-making. The analysis also showed that further levels in the structure did not add as much benefit as level 2 and that more costly information may be required to achieve significant improvements.

In the case of polymers, it was found that many classifications may account for the variation in the data, possibly because of less initial spread in the data or more challenges with data source error. Even so, similar level 2 performance as with the metals was seen in the polymers data. Once again by using a three part price grouping, approximately 45% reduction in uncertainty (excluding the more significant reduction from outliers) was achieved with 30-40% median error rates for all impacts except non carcinogenicity. The distinction rate was slightly higher at 94%. The taxonomy formation showed less improvement in the case of the polymers dataset, likely due to the aforementioned factors. Therefore, some datasets may not be as well suited to the type of analysis conducted in this thesis.

Lastly, the precious metals were grouped by material type and recycled content, which was very important for these high impact materials. The uncertainty reduction and error rates were similar to the polymers, except in the case of global warming potential, which had a slightly higher error rate. The distinction rate was even higher at 96%. The precious metals dataset showed a cleaner demonstration of the methodology with fewer materials and where data source was not a problem, albeit with smaller final groups. Akin to the metals, it also demonstrated that further improvement may be possible with more costly information that could distinguish between mining practices in different locations.

The materials taxonomies developed are designed to support streamlined life cycle assessment. By considering multiple environmental impacts, decision-making for multi-attribute environmental preference becomes more feasible. The next section will use the developed taxonomies and explore how the creation of effective structures allows us to improve our estimates of environmental impact

with less information. We will also consider our ability to make choices in comparative decision-making, which takes advantage of the efficiency of the structures, and their ability to distinguish between categories in a given level of the taxonomy.

4 Application of Methodology – Streamlining Case Studies

The data structures and list of key classifiers resulting from the methodology developed in this thesis are intended to support two types of streamlining applications. The first involves application of the hierarchical taxonomy to under-specification of a product bill of materials. This will be demonstrated in this section for a consumer product. The second involves the creation of prediction models, and two examples will be provided.

4.1 Examples of Under-specification

A consumer product consisting only of metals and polymers was selected for analysis with under-specification. This product was one of the products analyzed in the previous work by this research group (Patanavanich 2011). The product consisted of 36 components, where the largest component made up approximately 75% of the product's weight. Under-specification was used in three contexts: to assess the environmental impacts at different levels of specificity, to evaluate comparative decision-making in the case of materials substitution for the main component, and to determine the number of elements in the SOI using probabilistic triage.

4.1.1 Effectiveness at Different Levels of the Taxonomy

The consumer product was assessed at four levels of the hierarchy, which was developed in Chapter 3: level 1 consisted of only the groups metals and polymers, level 2 included categorization based on P1 (metals) and price (polymers), level 3 was based off the taxonomies shown in the next tier analyses in Chapter 3, and level 4 represented the individual database entries.

It is important to note in showing this case study that it is meant merely as an example. The analysis of the taxonomies in the previous section shows how well the structure works for all possible materials within the group, whereas a case study demonstrates only how well it performs for a select few. Thus, this is merely a demonstration rather than proof of overall efficacy.

The MAD-COV was tracked for each environmental impact and shown in Figure 4-1. In general, the values declined except in the case of global warming potential. This may have occurred because the largest component in the product is coincidentally in a group that has a higher MAD-COV for global warming potential at level 3 (P1-B-Other) than at level 2 (P1-B). This can be seen in Figure 3-19, where the highest point in the level 3 global warming potential plot is for the P1-B-Other group. On average we saw a decline in the MAD-COV from level 1 to level 4, but lesser gains from level 2 to level 3 as compared to level 1 to level 2, which is similar to previous results for the overall taxonomy discussed in Section 3.1.5.

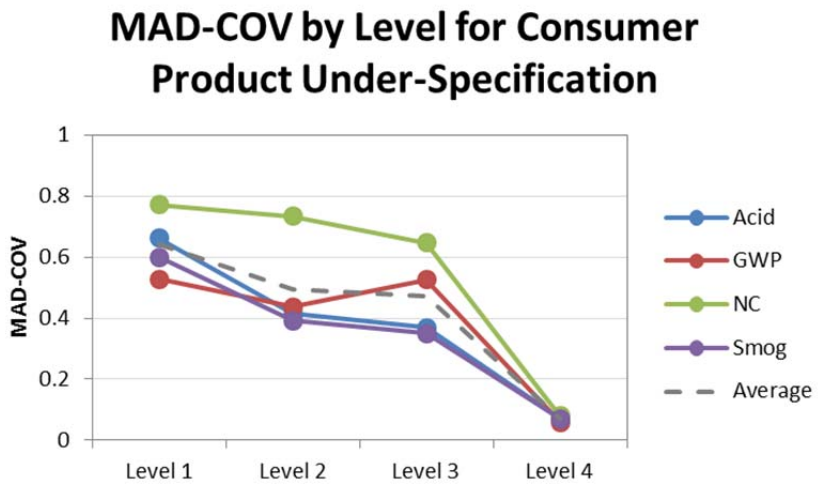

Figure 4-1. MAD-COV by level using under-specification

The MEDAPE decreased on average from 71% at level 1 to 56% at level 2 as seen in Figure 4-2. This effect was more pronounced in acidification and smog, but no improvement was seen for non carcinogenicity. Some additional decreases were seen between level 2 and level 3 for acidification and smog, but not for global warming potential and non carcinogenicity. Again, this may have been the result of the main component being in a higher variability group for level 3 as compared to level 2. The approximately 40% error seen for most environmental impacts at level 2 is somewhat reasonable considering that even well specified, best-practice carbon footprint studies have estimated uncertainties of 5-10% (Meinrenken et al. 2012).

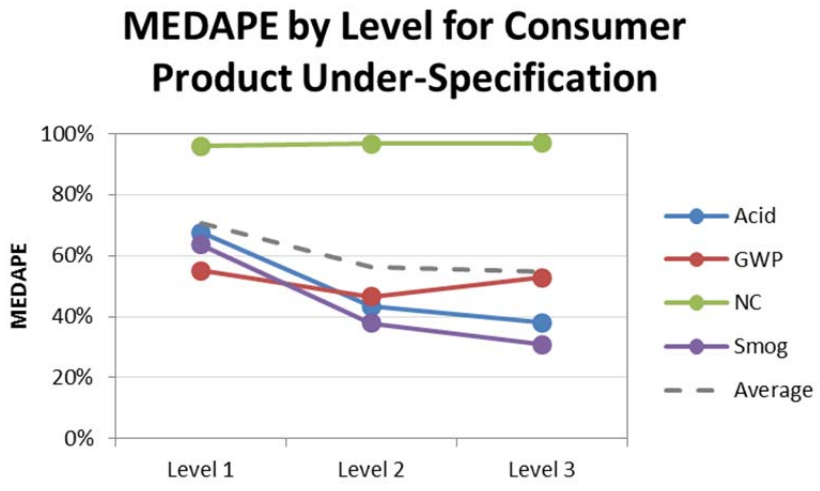

Figure 4-2. MEDAPE by level using under-specification

4.1.2 Comparative Decision-Making with Under-specified Data

One interesting decision-making question would pertain to whether or not we could tell which product was environmentally preferable when comparing two alternatives. To assess this, the main component (made from zinc) was substituted with two different options: 1) a material from P1-A at level 2 (low alloyed steel), and 2) a material from P1-B-Mg at level 3 (magnesium). The distinction rate, or the ability to determine the rank preference of the alternatives as defined in Section 2.4.2, was used as the comparator metric. The distinction rates were calculated for the comparisons at the level of specificity for which the categorization changed, which is level 2 and level 3 respectively (i.e., we would not be able to differentiate case 2 (magnesium) from the baseline at level 2, since both would be specified as P1-B, so we only evaluated it at level 3). The average value of the steel was lower in all impacts, and the magnesium was only higher than the baseline on average for global warming potential, which was a large difference.

The results from the analysis can be seen in Figure 4-3. In general, greater differentiation was seen when the group change was made at level 2 from zinc to steel. This makes sense since there is greater efficiency and differentiation between groups at this level. Except in the case of global warming potential, there was at least an 85% probability that the zinc product has a higher impact than the steel based product.

The product made with magnesium instead of zinc showed something slightly different. In this case, it was really only possible to choose an environmentally preferable product based on global warming potential, where there was 100% probability that the magnesium alternative had a higher impact. For the other impacts, the probabilities ranged from 52% to 66%, which were much closer to 50%. At 50%, it is impossible to tell which is environmentally preferable. The ability to only differentiate on global warming potential makes sense, because if we recall back to Figure 3-14, the magnesium metals only formed their own cluster based on differences in global warming potential. Thus, when multiple environmental impacts are considered, the reasons for the creation of certain groups within the taxonomy are important in understanding when product differentiation can be achieved for decision-making.

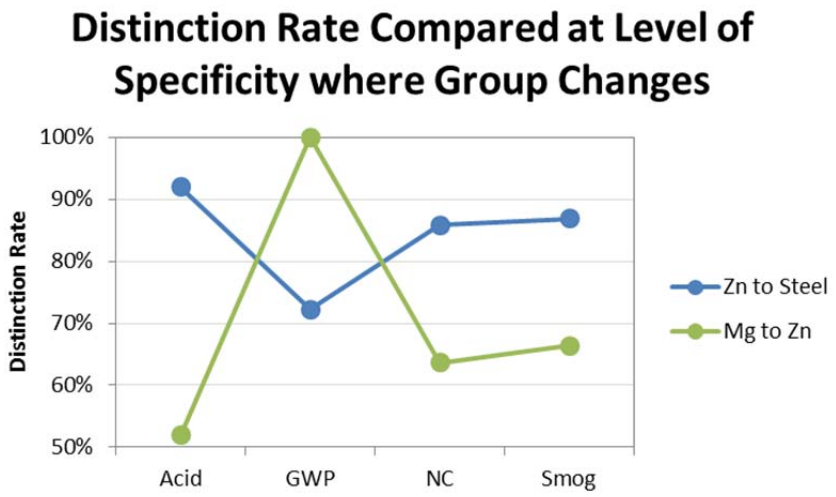

Figure 4-3. Distinction rate for comparison of products with one component changed from zinc to steel (compared at level 2) or magnesium (compared at level 3)

4.1.3 Identification of the Set of Interest Using Probabilistic Triage

The number of elements in the SOI was determined for the taxonomy at levels 1 through 4. The true SOI included one component for all impacts except global warming potential, which contained three components. The additional percentage of components (APOC) required to be specified at each level was calculated and the results are shown in Figure 4-4. When using data specified at level 1, an average of 24% additional components needed to be specified, whereas in level 2, this was reduced by more than half to an average of 10% additional components. Once again, little improvement is seen between level 2 and level 3. The reduction in components to be specified represents a theoretical cost savings in streamlining, since more detailed data collection is required for fewer product parts. This must be balanced with the additional cost of information from level 1 to level 2.

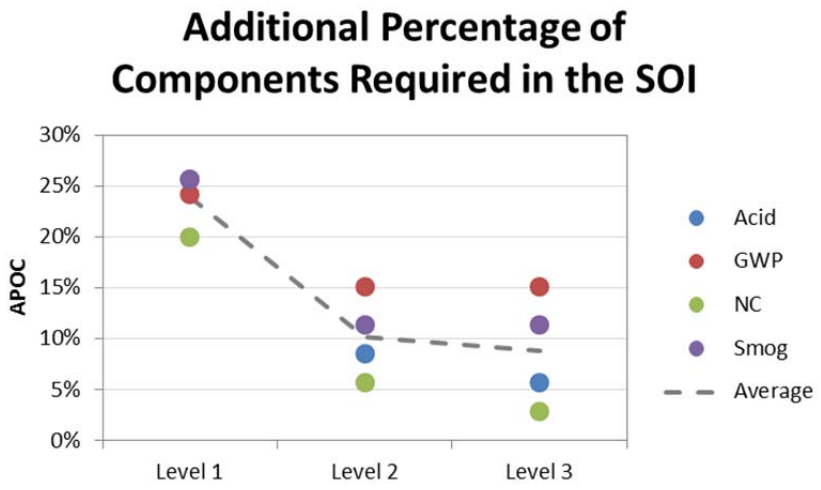

Figure 4-4. Additional percentage of components required in the SOI by impact and by level of specificity

4.1.4 Summary of Under-specification Examples

These examples illustrate how the materials taxonomy created in Chapter 3 can be applied using under-specification. More analysis of different case studies would illustrate strengths and weaknesses of a given taxonomy. In general in this example, the uncertainty, as illustrated by the MAD-COV, and the error rate, as illustrated by the MEDAPE, decreased as more information was provided across levels, with the most significant decrease between level 1 and level 2. These metrics may show different results depending on how well the materials in a given product are characterized in the taxonomy. Comparative decision-making was most effective when the categorizations were distinct across the range of impacts. Differentiation was possible at fairly high levels of significance for multiple impacts, even with specifying only the price ranges of the components. Lastly, adding a second level to the taxonomy enabled cost improvements in terms of the reduction of components required to be specified with more detailed data collection using probabilistic triage.

Although this analysis did not seek to compare taxonomies in under-specification, quick tests showed that improvement in the taxonomy effectiveness metrics translated to improvements in effectiveness when assessing the product as a whole using less specified data. When it came to using probabilistic triage for hybrids however, the effectiveness of a given taxonomy may be less relevant. This is potentially because the most important data are given at the highest level of specificity and any improvements in level 2, for instance, will only be applied to a small percentage of the data and impact. Thus, improvements may be too small to notice. More study may be useful to determine how different structures improve other factors, such as the number of components in the SOI.

4.2 Examples of Prediction Models

The classifiers can also be used for their predictive capabilities. In lieu of using under-specification as a means of quantifying impact when there are data gaps, impacts can be estimated using predictive models. A simple predictive model to evaluate is linear least squares regression. Two examples of using linear regression will be demonstrated here, based on classifiers identified in Chapter 3. One example will be shown for the metals dataset and one for the precious metals dataset. The polymers dataset was excluded from this part of the analysis due to the known challenges introduced by different data sources.

The response variable in these examples was based on the addition of the standardized log transformed environmental impacts, as in Section 2.3. Alternative response variables could include inventory values or specific impacts. However, since the goal here was to consider environmental profiles rather than specific values, this aggregated impact value was equivalent to an environmental indicator. The log transformation was necessary in order to create a fairly normally distributed variable for predictive purposes.

A stepwise regression procedure was used to test previously assessed classifiers and build a regression model. The stopping criterion for this procedure was the maximum five-fold cross validation R^2 value. This k-fold R^2 is reported for all models, and shows how well the model performs on validation data. Cross-validation made best use of the data available, particularly for smaller datasets like the precious metals.

Previous models showed that data source was an important classifier in the regression models, and that the variable was in fact significant. Data source may be useful for understanding differences within the data, but it does not provide much value in prediction. If a user is attempting to estimate an environmental impact, the data source does not exist, since the data does not exist. Thus, this classifier was excluded from the analysis, likely decreasing the performance statistics of the models developed. Future models could incorporate data source if a user would like to know an estimate of impact assuming it came from a specific data source.

Function and other categorical classifiers were translated into dummy variables so that they could be incorporated into the models. Outliers identified within the metals dataset (i.e., mercury and nickel from platinum group metal production in Russia) were also given a dummy variable.

The resulting models were evaluated for their R^2 values (from the model, the adjusted values, and the k-fold values), for the VIF values to determine effects of multicollinearity, and for patterns and normality of the residuals.

4.2.1 Predictive Model for Metals Dataset

The predictive model developed for the metals dataset showed recycled content, price, relative crustal abundance, and mercury to be significant classifiers. This is similar to the classifiers selected for the model in Section 3.1.3. Through the coefficients, we can see that higher recycled content decreased the environmental impact indicator while higher price increased it. Both of these effects were as expected. The relative crustal abundance however showed that as abundance increased, then the impact also increased. This was contrary to intuition that would suggest rarer materials would require more effort for extraction, and thus cause more environmental damage. This coefficient was likely a result of a correction after other factors had been incorporated. Price already accounted for some of the rarity and effort involved, and relative crustal abundance merely added a correction at constant price. The mercury increased the impact to a large degree as expected, likely due to the extreme nature of the outlier. However, the dummy variable for the nickel outlier was not found to be significant. The predictive model is shown by Equation 13.

$$ImpactIndicator = 0.16 + (-3.67) * RecycledContent + 1.42 * Log(Price) + 5.93 * RelativeCrustalAbundance + 3.93 * Mercury$$

(Eq 13)

The model showed a reasonable R^2 and explanation of the variation, as can be seen in Table 4-1. However, there was still some variation that was unexplained by this model. The validation results did show though that the model was robust to different data, as the k-fold R^2 was not significantly lower than the training value. All of the classifiers selected were significant at a 95% confidence level and they showed very little multicollinearity.

Table 4-1. Model statistics for predictive regression model for metals dataset

Metric	Value
R^2	0.7174
Adjusted R^2	0.7104
K-fold R^2	0.6530
VIF values	<1.1
p-values for explanatory variables	<0.04

Lastly, if we consider the predicted values compared to the actual values in Figure 4-5, we see fairly good alignment. However, there are a few points that deviated and may be contributing more to the unexplained variation. We see this again with the residuals. The residuals did approximate normality fairly well with some slight deviation on the lower tail. Overall, this model has reasonable predictive capability, but would likely need additional work to find even better parameters to consider for the residual uncertainty in order to achieve lower prediction error rates. This could result from more examination of the tiered exploratory analysis in Section 3.1.5 or additional process based information.

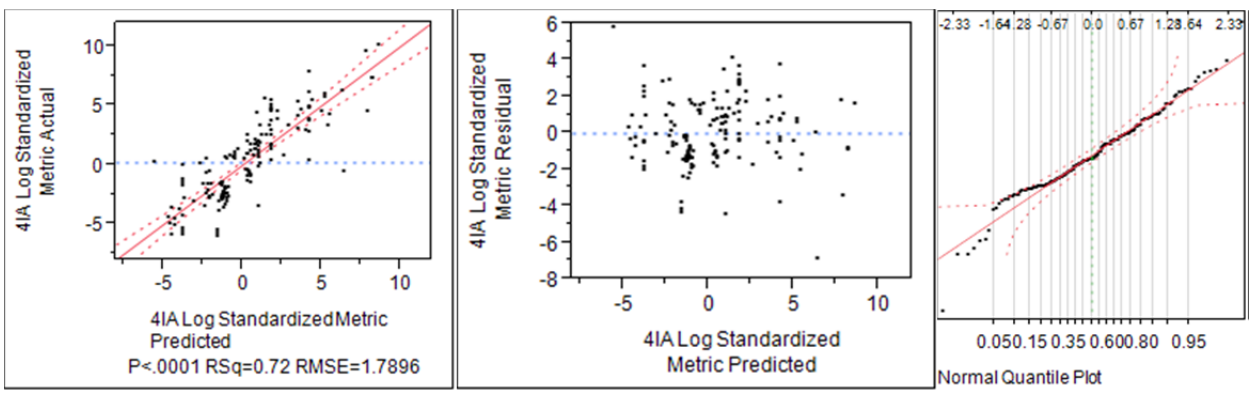

Figure 4-5. Regression diagnostics for predictive model for metals dataset. Predicted values compared to actual values (left), residuals compared to predicted values (center), and Q-Q normal plot for residuals (right).

4.2.2 Predictive Model for Precious Metals Dataset

The predictive model for the precious metals was fairly simple and similar to the one for the metals dataset. Only two of the classifiers were significant in this analysis: recycled content and price. They showed similar trends as the metals dataset and the sign of the coefficients were consistent with expectations. A dummy variable for silver metal was another possibility for an explanatory variable; however, it was not determined to be significant based on its p-value. The prediction model is illustrated in Equation 14.

$$ImpactIndicator = (-13.48) + (-6.59) * RecycledContent + 1.63 * Log(Price)$$

(Eq 14)

The model statistics for the precious metals dataset were stronger than those for the metals dataset. The R^2 was very high and the k-fold R^2 value once again supported the idea that the model was fairly robust across the data. All explanatory variables were highly significant and showed little multicollinearity. One explanation for the improved R^2 values is that this dataset was not confounded by data source challenges.

Table 4-2. Model statistics for predictive regression model for precious metals dataset

Metric	Value
R^2	0.9252
Adjusted R^2	0.9207
K-fold R^2	0.9092
VIF values	~1
p-values for explanatory variables	<0.0001

Considering the predicted versus actual values in Figure 4-6, we see that there are two main clusters of the data. This was consistent with all of the previous exploratory analysis. However, it does not make for a great linear trend, since likely more data would add localized scatter rather than fill in intermediate values. The large value differences between the two groups made this approximation appear more significant than it is. The residuals were in two main lines since the values do not vary sufficiently for a typical residual plot. They did however approximate normality very well. In general, this model seems to have reasonable predictive abilities, but is challenged by the low number of data points, potentially distorting its quality. Other types of predictive models that can segregate the two data clusters may be better suited for this dataset.

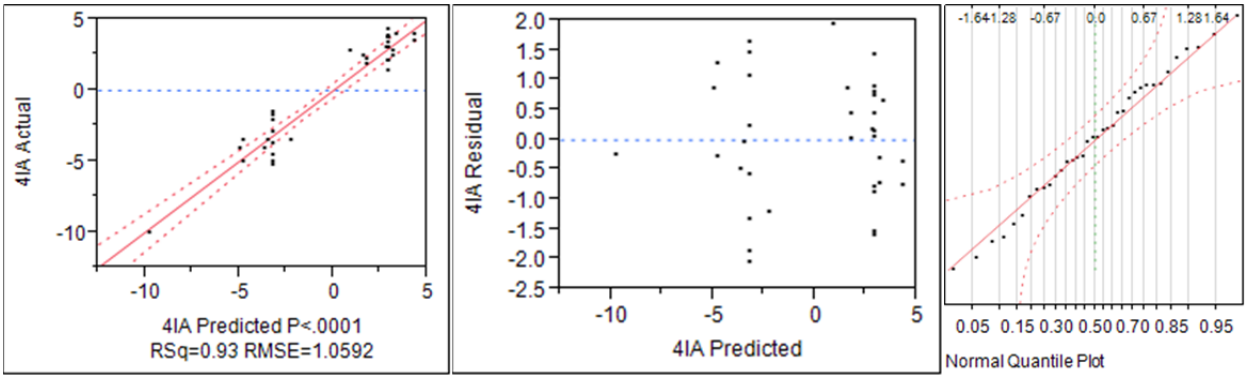

Figure 4-6. Regression diagnostics for predictive model for precious metals dataset. Predicted values compared to actual values (left), residuals compared to predicted values (center), and Q-Q normal plot for residuals (right).

4.2.3 Summary of Predictive Models

These models provide a simple example of how the classifiers identified could be used to create predictive models. They highlight a few interesting characteristics. One is the importance of factors that account for residual uncertainty in the data. Although, the analyses in Chapter 3 are able to ascertain classifiers contributing to the main sources of uncertainty, more work is necessary to identify these supplemental factors. This could be achieved with more exploration into the principal components (i.e., PC3 and PC4) or with more focus on next tier clustering analysis and exploration.

Regression models are a fairly simple approach to prediction. Other methods could also be applied to possibly achieve higher predictive capabilities. The regression trees are one option, although often they require a large number of characteristics that must be known, which might add to the cost of the analysis. Other models such as hierarchical models or neural network models might provide value as well. Neural network models have been successfully used within the LCA space both for product level prediction and for prediction of the environmental impacts of chemicals (Sousa et al. 2000; Wernet et al. 2008).

5 Discussion

This thesis applied data mining methods to explore classifiers useful for the creation of hierarchical classification structures and prediction of environmental impacts. This work considered the environmental profiles of three material types. Results showed the use of classifiers for taxonomy development that were able to improve effectiveness over structures in the previous work at high levels of efficiency. It was seen that the methods applied were able to help address some of the primary drivers of the uncertainty within the data and reduce prediction error rates. This section will consider the reasonableness and implications of the results presented. This will include discussion of the classifiers identified and their reasonableness, the effects of looking at an environmental profile rather than an individual impact, the limitations and challenges of this method, some possible application areas, and opportunities for future work and development.

5.1 Classifiers

The main classifier identified as significant was the price. Others included the function, recycled content, relative crustal abundance, maximum service temperature, and material type. Price in particular seems to be a fairly reasonable indicator of the environmental impact, as it may be related to the amount of effort required to extract and process a material. This might be in terms of energy or chemical use, which can be directly related to some of the environmental impacts. In the case of toxicity, materials that are regulated for toxicity factors (e.g., additional safety requirements, disclosure, etc.), have regulatory requirements that could increase its cost in line with its environmental damages. This is how price can be related to many environmental factors. Indeed, Meinrenken et al. also used price as a predictor variable in their environmental footprint metric (Meinrenken et al. 2012).

There are of course exceptions to this. For instance, for high technology materials where intellectual property plays a role, price may be distorted. Intellectual property was less of a problem in this assessment, since these datasets represented more common materials. Another exception is in the case of recycled precious metals. For those materials, there is no discounted price for using recycled materials, while there is significantly less environmental burden. The scarcity rent associated with the precious metals distorts the price beyond the environmental damages. Thus, from a taxonomy perspective the price was less useful for precious metals. However, where we can account for recycled content in addition to price, such as in the prediction model, categorization may be useful. A final example of where price may not correspond to environmental impacts is in cases where the emissions are a result of low cost (and higher environmental impact) substances, because the material is not regulated to a degree where it would account for the environmental impact. This is the case for mercury, which has a very severe non carcinogenic effect not accounted for in the price.

It is also important to note that this analysis was conducted in terms of a manufacturer's perspective rather than a consumer's perspective. If the price was examined at a consumer level, this would introduce additional uncertainty factors into the cost, such as the influence of intellectual property or brand. Costs from a producer perspective are much less variable, as there are fewer value added steps to distort the price. There may be some variability introduced though due to processing of the materials, depending on the scope of the producer's operations.

Other factors such as function are an aggregation of identified classifiers, and thus it is reasonable that function also appeared as a potential classifier. For metals, function may be related to the level of purity

(and therefore processing) which is required and may also be related to the rarity of the materials. In the case of the polymers, function may be related to temperature properties and price. Again, there will be exceptions to the relationship between function and environmental impacts, as there are substitutable materials with significantly different environmental profiles. However, in general, more advanced applications can typically require more effort to produce the materials.

Quantitatively identifying recycled content as a classifier is intuitive, since in general recycled content will significantly reduce the amount of energy required in processing, which will in turn have direct effects on the overall environmental burden. Another classifier, service temperature, may be related to the energy required for processing or for reactions to produce the material and therefore, may also be intuitively related to environmental impacts. Lastly, relative crustal abundance may have an influence on the ease of extraction of metals, and so again represents a reasonable classifier. Crustal abundance in this analysis was generally correlated with density, which was another factor utilized by Meinrenken et al (Meinrenken et al. 2012).

In addition to the classifiers, a number of outliers were identified. The outliers for mercury and PTFE were also identified in the regression analysis performed by Huijbregts et al. They explained these outliers due to HCFC-22 emissions for the former and mercury emissions for the latter (Huijbregts et al. 2010).

In terms of "knowability", the function and price are fairly easy for a manufacturer to know. When using a part in a given product, the function of the part will be known and the price paid to obtain it will also be known. Thus, it is useful that price was an influential factor, since this information is readily obtainable. One factor that is challenging with price though is that it is an emergent property rather than a physical property. Over time it can change and it may be variable based on external factors previously mentioned that are unrelated to environmental factors. Thus, even if the taxonomy is designed appropriately, there may be some misclassification errors when a price is near the threshold values between categories or is variable. For users who are concerned with challenges related to price, function may be a reasonable substitute, although as we saw, it does not have quite the same effectiveness.

In terms of consistency across material types, the price classifier was fairly consistent across the categories explored, with the noted caveats for precious metals. It is useful to have a single uniform classifier for an overall taxonomy, as it targets data collection for the user to one type of information for

all materials. Supplemental classifiers were material type specific though. Thus, it is useful to analyze the types separately to provide insights for predictive models for instance, but uniformity may suffer in these cases.

There are a few implications of the fact that price was observed to be the most important classifier overall. In general for these materials, price was directly related to environmental damage factors. Thus, the distortion of market energy prices may affect the ability to take those factors into account. However, as was noted, it may be beneficial to distort traditional market dynamics in other ways to enhance the relationship with price, such as with toxic materials or other factors where the price is not directly related to the environmental impact on its own. This would allow the alignment of financial and environmental decision-making.

5.2 Effects of Looking at Multiple Impacts

The environmental impacts that were selected for analysis do have an impact on the results obtained through this method. As indicated previously, the inclusion of new impacts means new outliers and influential points must be considered in the structure creation. Since these influential points will not always be ranked the same across all of the impacts, as more impacts are included, more groups may need to be formed at a given level to achieve the same effectiveness. This is because reducing error within one impact can increase it in another. One example of where an additional group must be formed comes from the precious metals. With the incorporation of smog formation, the gold needed to be separated from the platinum group metals to reduce the overall error rates and uncertainty. Similarly in the second tier analysis for metals, the copper was higher in acidification and/or smog formation, while magnesium was higher in global warming potential. Considering only a single impact would not have required so much segregation of material types at this level.

Due to the complexity of considering multiple impacts and the multivariate analysis, visual observation is difficult when more than one impact is considered. For one impact, a rank analysis can simply be conducted and material groupings made accordingly. When considering multiple impacts, grouping by rank analysis for one impact may lead to high levels of variability in other impacts.

Examination of certain impacts can be more challenging than others. For instance, human health non carcinogenicity can be more difficult to analyze using this methodology, and it starts with a higher level of uncertainty. Part of the reason for this might be due to poor data quality within this metric such as from the lack of trace emissions data or lack of appropriate models to characterize all toxic compounds (Huijbregts et al. 2010). Thus, with data problems in the individual process data, it will be difficult to identify consistent patterns and useful classifiers. Further challenges in identifying classifiers for non carcinogenicity may come from the large number of elementary flows that drive this impact assessment method as compared to others. Thus, more factors and classifiers may need to be determined to fully assess and reduce the uncertainty in this category.

Lastly, it is theoretically possible to analyze the data at the inventory level instead of the impact level using this methodology. The inventory level has many more variables (i.e., elementary flows) to assess in a multivariate analysis. This may exacerbate some of the concerns listed above, such as poor data quality in individual elementary flows or the requirement of more groups when considering the multivariate versus the univariate space. It may also create data sparsity issues, which has been

previously discussed, but may be able to be addressed through the methods described or by identifying key elementary flows. Thus, although this would provide a more ideal representation of the environmental profile without the additional uncertainty incorporated by impact assessment models, it does create some challenges that should be considered.

5.3 Limitations and Challenges

While this method has shown the ability to reduce the error rate in streamlining particularly between a general materials category and one with a bit more specificity (i.e., level 1 to level 2 as described above), there are some challenges and limitations that should be discussed.

5.3.1 Data Quality

The first challenge relates to the data quality. The datasets do not actually represent a randomly sampled population of the possible materials and their environmental impacts. There are missing data elements and the distribution is not directly representative of the materials in use in society. This can lead to some deviations in the importance of certain classifiers. However, we chose to work with the data that were available through LCI databases rather than perform data collection activities, and opted to use data commonly used for secondary data in LCA.

Data source error has been another theme discussed throughout this thesis. It unfortunately limits the ability to gain insights. This was especially true in the case of the polymers, where the data had lower original variability, and so the data source was a relatively large contributor. Data source error was also a major challenge when considering certain environmental impacts. One of these was ozone depletion potential. The source of the data could be very clearly delineated when observing the visualizations of the data for this impact.

These challenges identified have ramifications for the field as a whole. As comparative evaluation of products becomes more mainstream along with use environmental product declarations, these data quality factors remain hidden in the background. If data source is so influential in certain questions, this implies the need for stricter standardization requirements and data quality standards in order to enable these product comparisons.

5.3.2 Structure Creation Challenges

In addition to the challenges related to the data quality, a few other difficulties exist with the methodology. Although the methodology provides a high level of simplification after application, it does require a high upfront cost in data collection and analysis. Many different attributes needed to be assessed in order to determine which were the most valuable descriptors. Along with this, the limited availability of experts could affect the application of the methodology. As expert judgment is an important part of the exploratory analysis in identifying key classifiers, the experts that were consulted may play a role in the conclusions reached. For instance, in this work, it is possible that different experts

may have been able to identify better descriptors, particularly in developing level 3 of the taxonomy and beyond.

The models have also been trained on a given set of data. Thus, as new data became available, particularly for materials not previously included within the dataset, they would have to be evaluated for whether they could fit into the frameworks created. New materials may not follow the same trends, and should be considered cautiously.

This methodology suggests many possible taxonomies. The results discussed some of the trade-offs between different metrics evaluated for effectiveness and efficiency. These metrics do not always align, and so it can be difficult to identify the "best" structure. This creates some challenges if the goal is optimization or showing that one structure is superior to another. However, it does also provide the benefit of flexibility for users. By illustrating multiple possible structures that show improvements in these metrics, users may be able to choose one best suited to their needs and based on the data available to them. Every user will not necessarily want the same type of structure as every other user for their end application. For instance, if users only use low impact materials, those structures that quickly segregate out the low impact materials rather than the high impact ones may provide more value to them in reducing the uncertainty of their under-specified data. User needs could also affect which metrics are useful to report, depending on how they would incorporate the taxonomies into their streamlining process.

5.3.3 Metrics

It was difficult to determine an appropriate effectiveness metric to assess the data. Many studies focus on coefficient of variation (COV) as a metric. However, this is misleading in the case of skewed datasets. In this work, two metrics for representing uncertainty were discussed: the MAD-COV and the SSW/SST. These two metrics showed different results for the taxonomies. For instance, in the case of metals, using the SSW/SST metric, P2 seemed to be the most promising candidate, whereas with the MAD-COV, P1 was the most effective. Furthermore, with the MAD-COV, one poorly characterized group, even if it is beneficial to separate out and should have lower relative uncertainty (e.g., PVF), may have a higher MAD-COV than the baseline and thus appear problematic. With these challenges with the uncertainty metrics, optimization and selection of "best" taxonomies is difficult. Metric development presents an opportunity for future improvement in this methodology.

5.4 Possible Applications

This work was very effective at analyzing data overall and identifying problematic data. This included identification of outlier points that should be examined for data quality. The methodology developed in this thesis was also effective at identifying data that were problematic for other reasons. For example, in initial iterations with the clustering analysis, a database entry based on an incorrect functional unit was erroneously included. Examination of the clusters easily identified this as a problematic database entry, and so it was then excluded. The analysis was able to identify incomplete database entries to be excluded as well. This identification of data challenges extends to the problems with data source. The methodology is able to show where data source is more problematic, and thus target areas for future data improvement or standardization efforts.

The taxonomies presented in this work are able to be used for streamlined assessment via under-specification. An example of this was shown for a simple consumer product application, and it was demonstrated that the uncertainty in results decreased as more information was provided. Differentiation was also possible depending on the impacts under consideration and the level of specificity provided. Furthermore, cost reductions in triage type streamlining methods were feasible due to lower detailed data collection requirements, although cost of data collection must also be considered.

Although the premise of this work suggests that structured data are preferable to proxy data, another potential application of this work is in guidance for proxy selection. Information from the classifier evaluation can assist in proxy selection. For instance, since price and recycled content seemed to be important factors, if one were to choose a substitute database entry, one should ensure that these factors were similar in the target process and in the proxy chosen. This type of analysis can be further developed to provide more guidance into criteria for proxy selection.

Lastly, this work can be used to inform the development of predictive models. Similar to the guidance for proxy selection, the classifiers identified can be used to create prediction models, such as neural network type models. A simple example of this was demonstrated with regression models to show models with reasonable predictive abilities.

5.5 Future Work

In the future, more work is necessary on metrics development. This may include algorithm development to determine the most appropriate classifiers, or may involve work with users to understand which classifier information would be most available. This work did not include an exhaustive look at data mining methods, so others, such as hierarchical modeling, could be considered.

This work can be expanded in a few other ways as well. First, it can be applied to more material types to create a comprehensive taxonomy. New insights will potentially be derived from exploring additional material types. Secondly, more development is required to identify improved level 3 classifiers, as these were shown to be insufficient to capture the full variation in the data. Thus, there is an opportunity to dive deeper into the data to identify what appropriate classifiers would be and to work more with experts to develop this understanding. Additional study can help understand the drivers for why the classifiers identified in this thesis appeared significant and the relative costs of acquiring information on classifiers.

For under-specification, the relationship between the effectiveness and efficiency metrics for taxonomy development evaluated in this thesis and under-specification performance factors (i.e., effectiveness at levels of the taxonomy, comparative distinction rates, and SOI counts) can be explored more thoroughly. This will help in understanding how significant improvements in the structure must be to benefit this type of streamlining application.

Lastly, the predictive model capability can be expanded. This work has created a framework for future development within this space and identified some useful parameters to include in predictive models. There is an opportunity to further explore classifiers that capture lesser parts of the variation or to create more advanced predictive models.

6 Conclusion

Materials taxonomies, and data structures more broadly, provide a simple and intuitive means of streamlining life cycle assessment. Requiring relatively low cost information, they offer a structured way of incorporating uncertainty into an assessment and allow for useful environmental decision-making strategies. This research showed that quantitative methods are helpful in creating effective and efficient structures, particularly when multiple environmental impacts are considered. This provides a viable option for secondary data specification or streamlined decision-making. However, process data quality and boundary assumptions, particularly related to the data source, remain a challenge that inhibits the ability of quantitative methods to discern meaningful classifiers in the data. Further work is needed around metric development to optimize taxonomy development and selection.

This research found that, in general, price is an effective and efficient means of classifying materials, particularly for the polymers and metals datasets. This is a useful finding, since price is typically an easily knowable characteristic from a manufacturer's standpoint. The precious metals represent an exception to the price categorization, however, and indicate that recycled content may also be very relevant within that dataset. Furthermore, although price performed the best for metals and polymers in this analysis, many classification methods did show significant improvement over level 1, often close to price, indicating that other options are viable, depending on the data available to a given user.

For the selected classification methods, significant improvements in effectiveness were possible with very few groupings. The proposed classification structures had five groups for each material type analyzed. For metals, a 55% reduction in variation was possible as measured by the within sum of squares (SSW). For polymers (excluding outliers) and precious metals, this value was approximately 45%. The median percent error for the taxonomies for all materials was approximately 30-40% for all impacts except non carcinogenicity, which was 65-80%. The uncertainty in the groups in terms of the weighted median absolute deviation coefficient of variation (MAD-COV) across materials was 30-45% for all impacts except non carcinogenicity, which was 65-90%. The precious metals exhibited lower uncertainty, and the metals generally had higher uncertainty. These relatively low error and uncertainty rates were achieved at the same time as high efficiency, shown by distinction rates over 90%. Thus, the development of effective and efficient structures is possible, and classifiers can be used to describe the data to a reasonable level. Attempts to progress the analysis to further taxonomy levels showed lesser improvements, indicating that perhaps either actual variation in the data limited the reduction or alternative classifiers might be required, which may be more costly.

The under-specification case studies showed the efficacy of the taxonomies for analyzing the data at lower levels of specificity and reducing data collection costs. The first under-specification example showed that providing more information generally improved the effectiveness and error rates of the estimated values. For all impacts except non carcinogenicity, both measures were reduced to approximately 40% using level 2 of the taxonomy. Thus, this can be useful for quick assessments or with secondary data.

The second under-specification example demonstrated that even with specifying minimal information about price (i.e., low, medium, and high for a given material type), an efficient data structure can allow for selection of an environmentally preferable alternative. The probability that the correct choice was made at level 2 ranged from 72-92%, with only one impact below 85%. More study can be undertaken to understand the limitations of the structure in achieving high distinction rates.

The third under-specification example demonstrated that incorporating an additional level to the taxonomy (i.e., level 2) was able to reduce the number of components required for specification in probabilistic triage by half. This reduction enables cost savings by significantly limiting the number of components requiring detailed data collection, although does require some additional generic data collection (i.e., approximate price) on all components.

Lastly, the predictive models provide a demonstration of how the classifiers could be used to fill data gaps through an alternative method. Four classifiers identified through the data mining methods were able to predict the aggregated environmental impact of the metals and account for 65% of the variation in the data. For precious metals, 91% of the variation was accounted for with only two classifiers. More exploration is required to understand the residual variation in the metals data.

In terms of the final question posed at the outset, we found that consideration of multiple environmental impacts created additional challenges in the development of data structures. A structure that decreased uncertainty for one impact could result in increased uncertainty in another. Also, the introduction of more impacts meant that more data points became influential in at least one impact, and so more groups were required in the classification structures to maintain the effectiveness of the structure as a whole. Systematic implications of examining multiple impacts can be studied in the future.

As streamlining efforts continue to gain prominence and aid scalability of life cycle assessment, this methodology can cost effectively help improve resolution of environmental impacts. Furthermore, with improving data quality, this type of exploratory data analysis will prove more useful in identifying key classifiers driving data variation and may also be beneficial in screening for data quality.

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8 Appendix A: Classifier Evaluation

8.1 Metals Classifier Evaluation

Principal component analysis showed some correlation between recycled content and price and PC1. It also showed some distinction between groups based on function and ferrous vs. non-ferrous metals categorization.

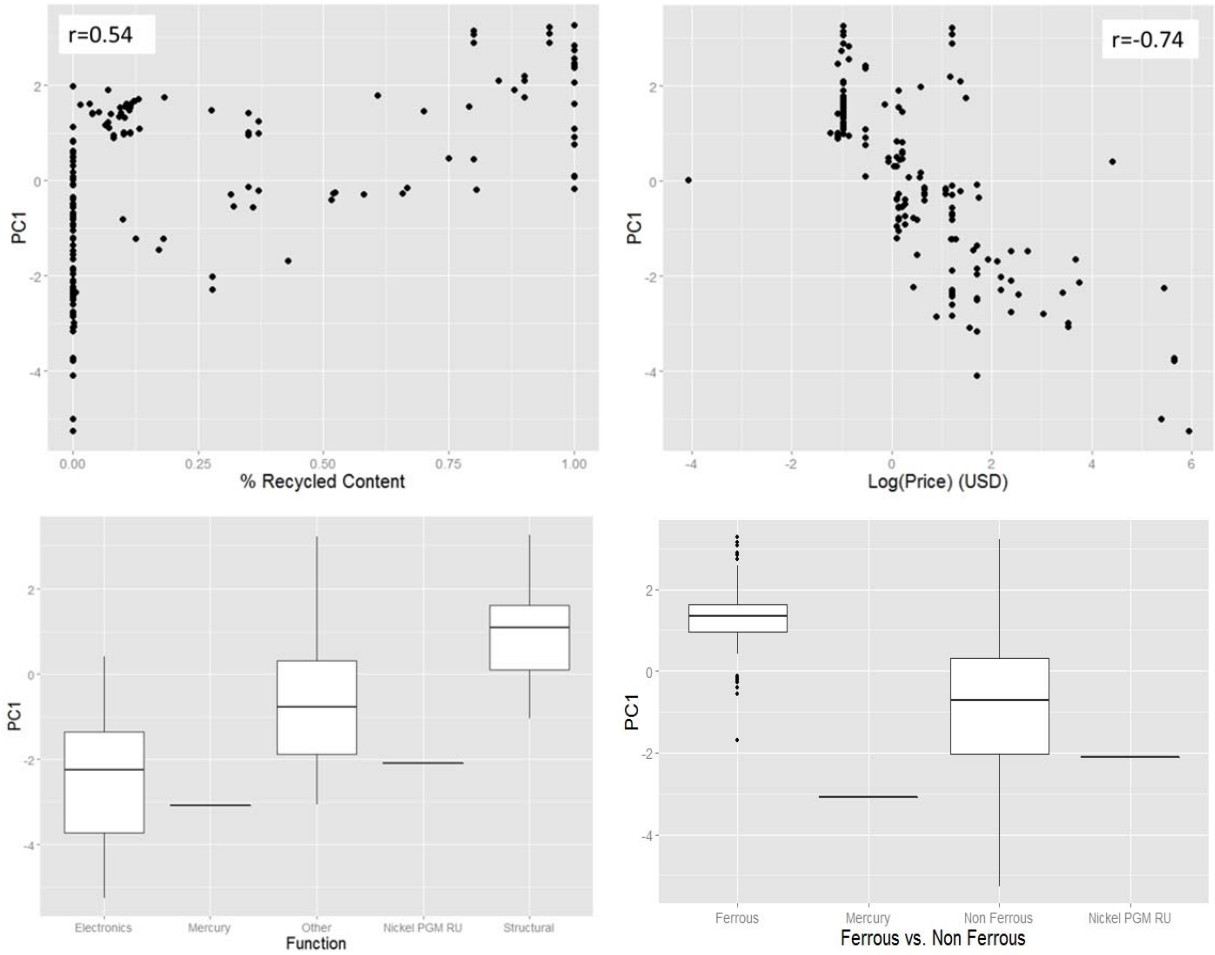


Figure 8-1. Relationships between continuous and categorical classifiers and PC1 for the metals dataset

The predicted vs. actual values and residual plots for the best regression model developed in the metals classifier evaluation are shown in Figure 8-2.

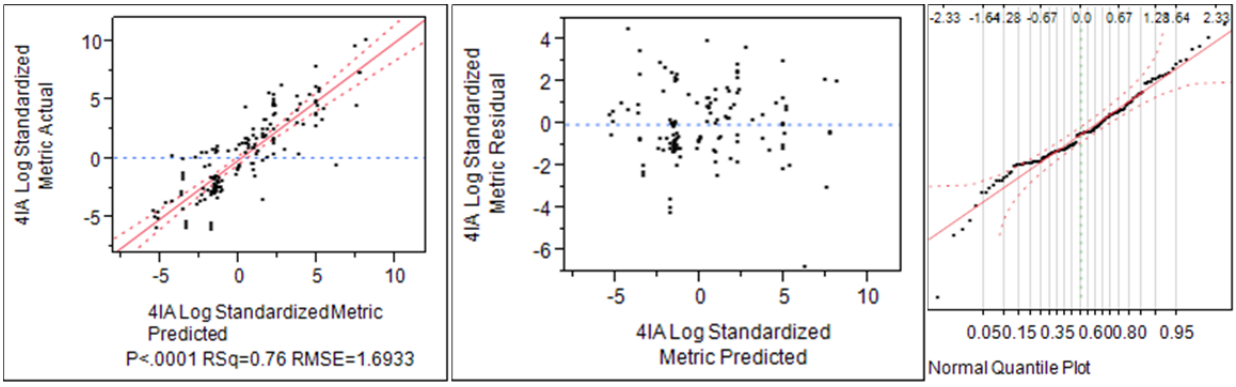


Figure 8-2. Regression diagnostics for classifier evaluation for the metals dataset. Predicted values compared to actual values (left), residuals compared to predicted values (center), and Q-Q normal plot for residuals (right).

8.2 Polymers Classifier Evaluation

Principal component analysis showed some correlation between maximum service temperature and price and PC1. It also showed some distinction between groups based on the percent fluorine in the repeat unit.

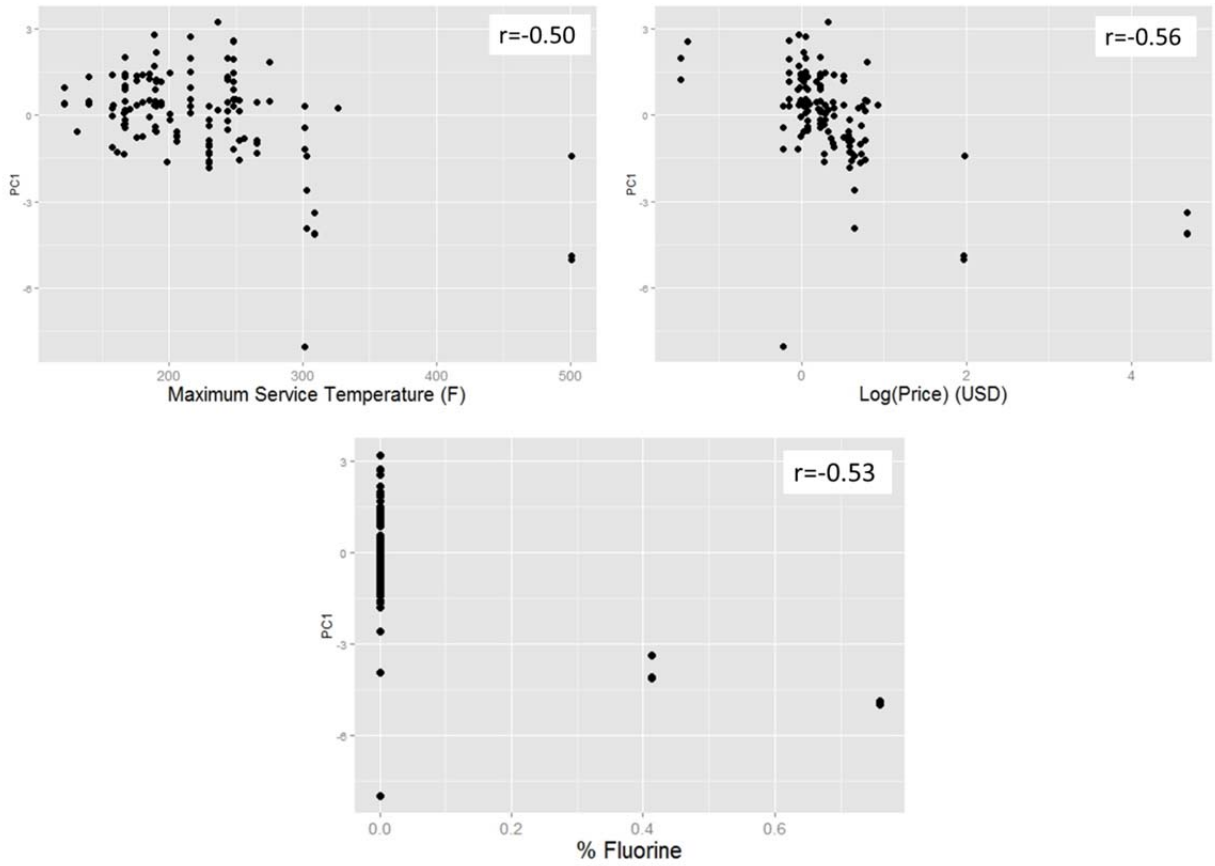


Figure 8-3. Relationships between continuous classifiers and PC1 for the polymers dataset

The predicted vs. actual values and residual plots for the best regression model developed in the polymers classifier evaluation are shown in Figure 8-4.

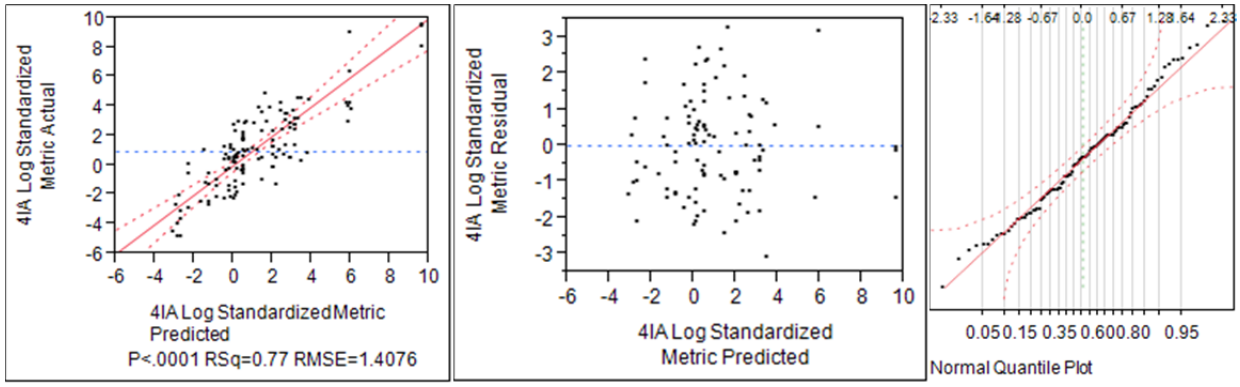


Figure 8-4. Regression diagnostics for classifier evaluation for the polymers dataset. Predicted values compared to actual values (left), residuals compared to predicted values (center), and Q-Q normal plot for residuals (right).

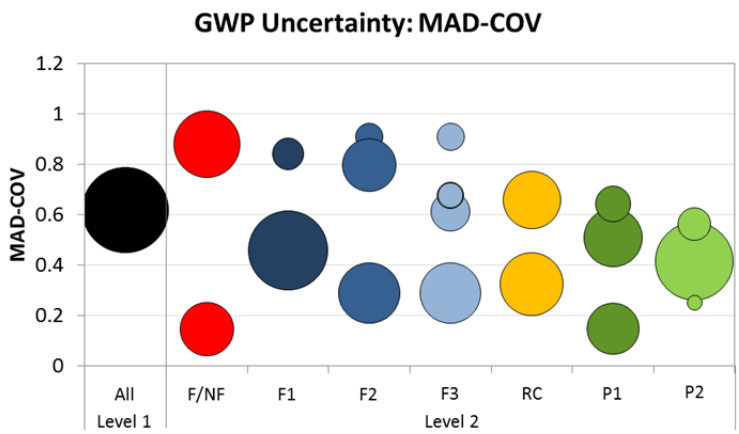
9 Appendix B: Taxonomy Formation

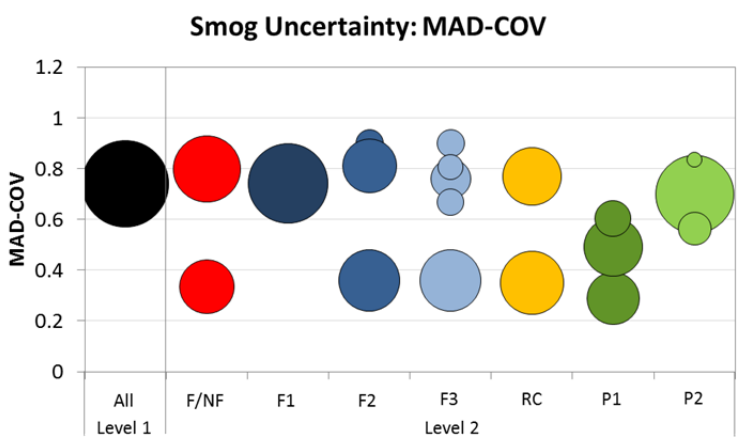
The following plots display the MAD-COVs for each group in a proposed taxonomy. Unlike the plots in Chapter 3, each group is displayed as a bubble, where the size of the bubble represents the number of elements in the group.

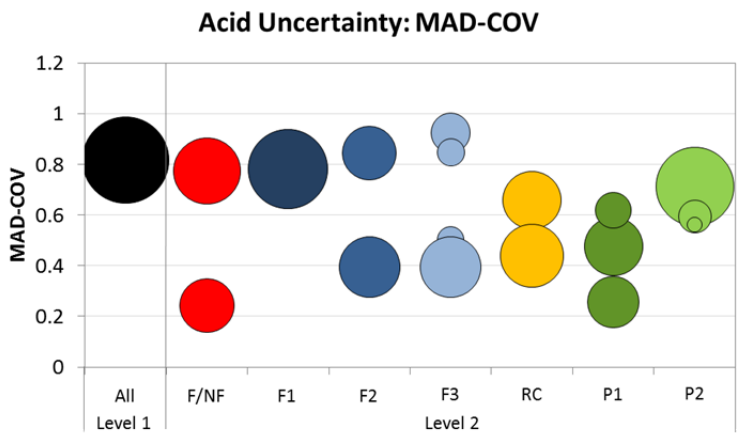
9.1 Metals Taxonomies

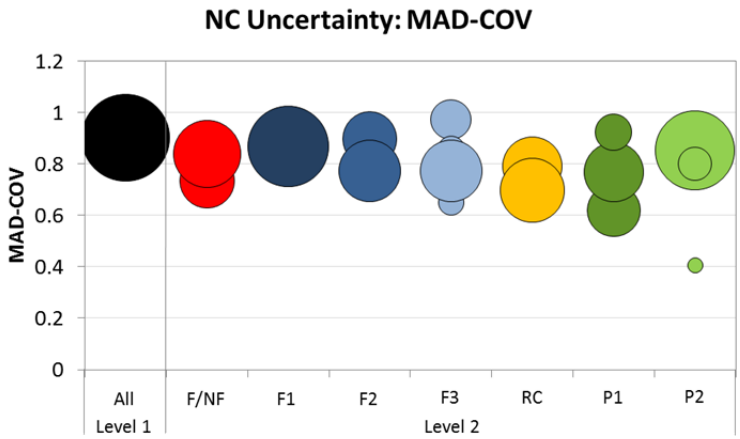
9.1.1 Level 2 Proposed Taxonomies

These plots show the MAD-COVs for the proposed level 2 taxonomies described in Section 3.1.4.



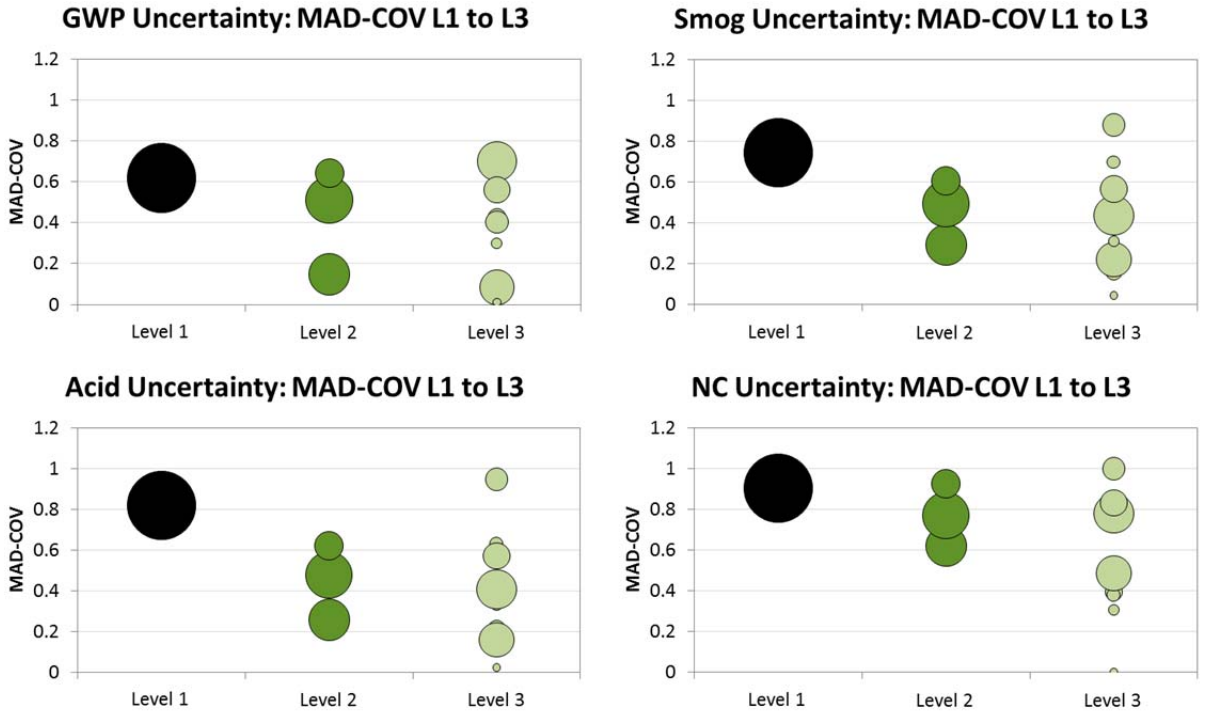



Acid Uncertainty: MAD-COV
MAD-COV
1.2
1
0.8
0.6
0.4
0.2
0
All
F/NF
F1
F2
F3
RC
P1
P2
Level 1
Level 2


NC Uncertainty: MAD-COV
MAD-COV
1.2
1
0.8
0.6
0.4
0.2
0
All
F/NF
F1
F2
F3
RC
P1
P2
Level 1
Level 2

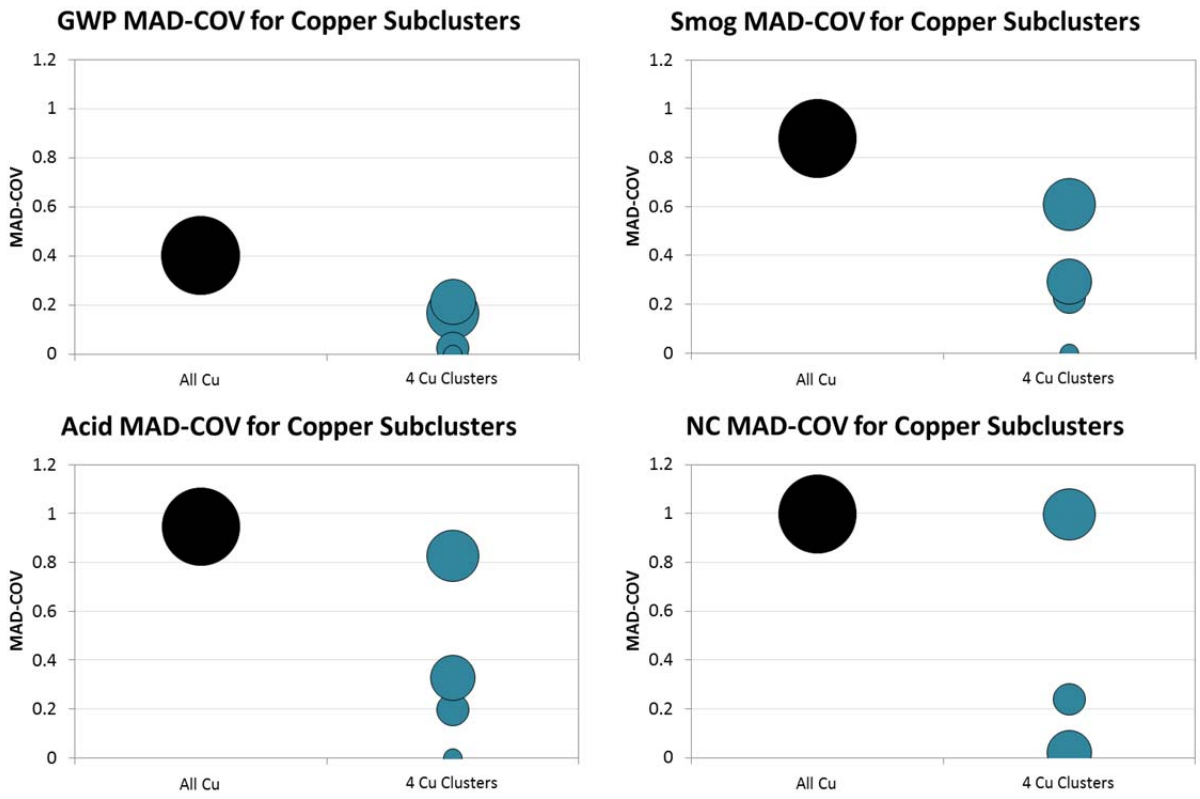
9.1.2 Level 1 to Level 3

Level 1 includes all metals database entries, level 2 is based on P1, and level 3 is based on the taxonomy described in Figure 3-16.



9.1.3 Copper Only

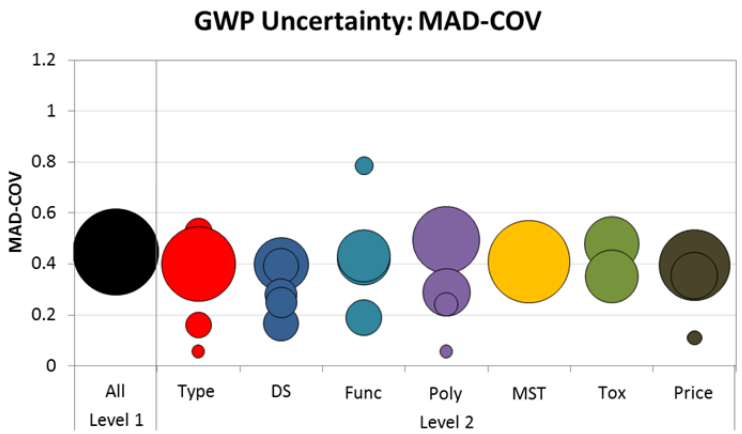
These plots show the MAD-COVs for the copper cluster as a whole and when it is broken into four groups as described in Section 3.1.5.

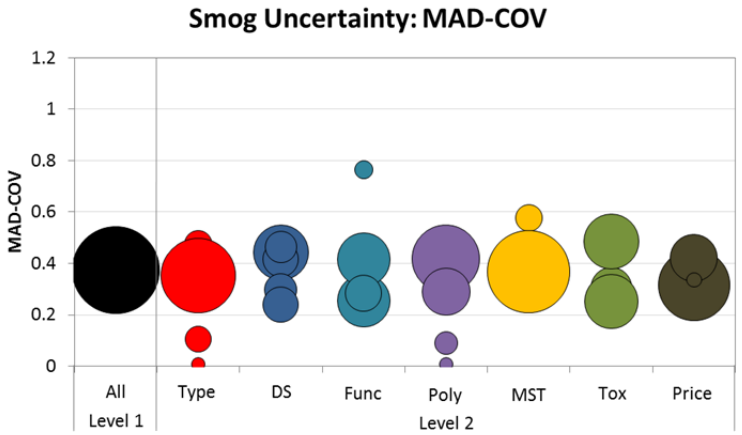


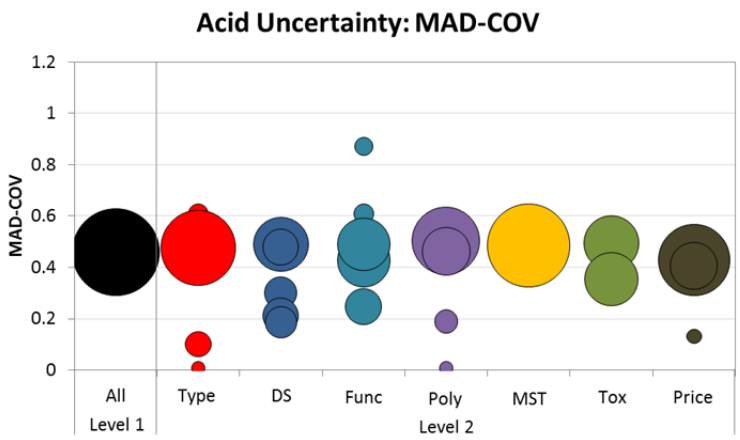
9.2 Polymers Taxonomies

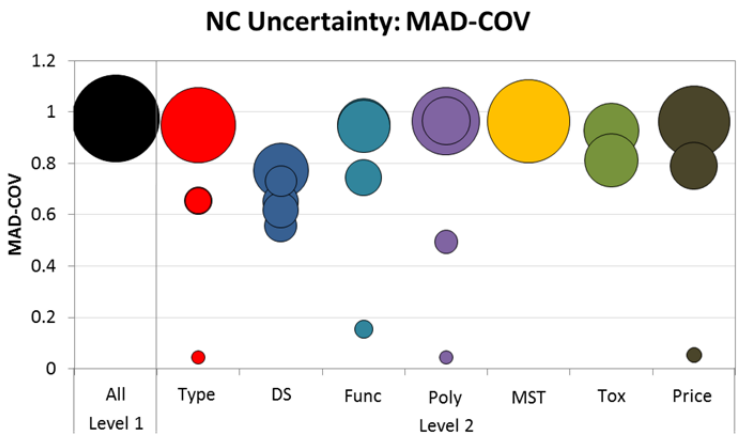
9.2.1 Level 2 Proposed Taxonomies

These plots show the MAD-COVs for the proposed level 2 taxonomies described in Section 3.2.4.



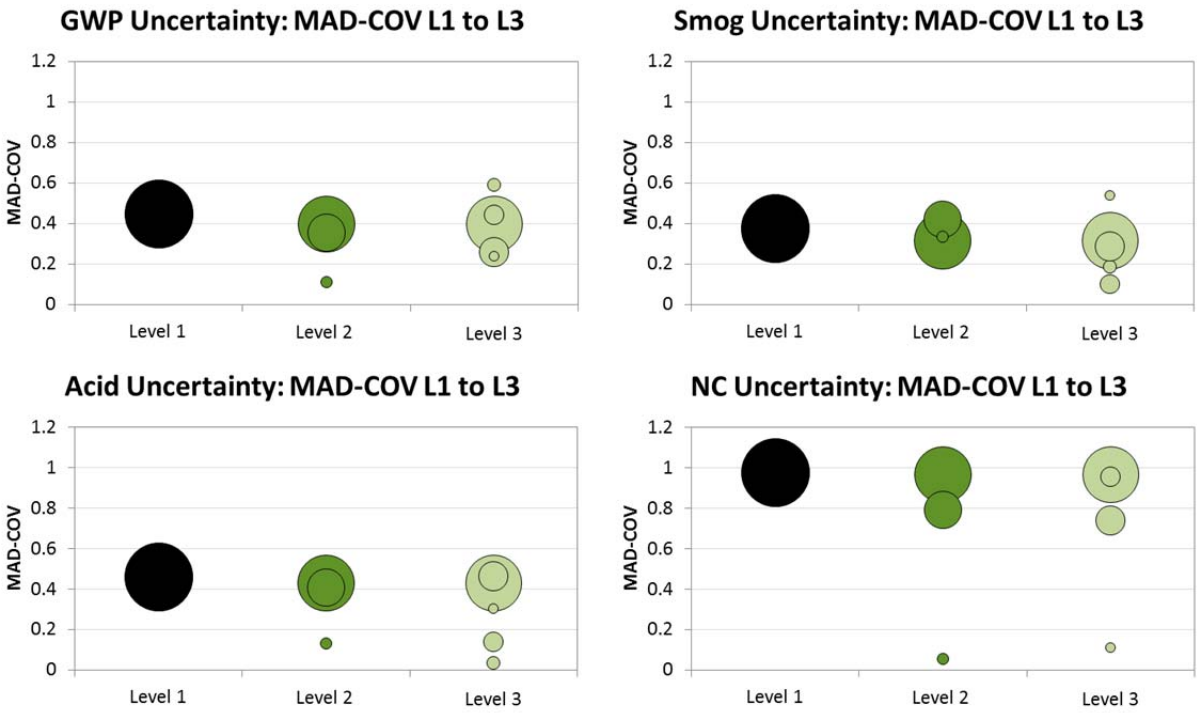



Acid Uncertainty: MAD-COV
MAD-COV
1.2
1
0.8
0.6
0.4
0.2
0
All
Level 1
Type
DS
Func
Poly
MST
Tox
Price
Level 2


NC Uncertainty: MAD-COV
MAD-COV
1.2
1
0.8
0.6
0.4
0.2
0
All
Level 1
Type
DS
Func
Poly
MST
Tox
Price
Level 2

9.2.2 Level 1 to Level 3

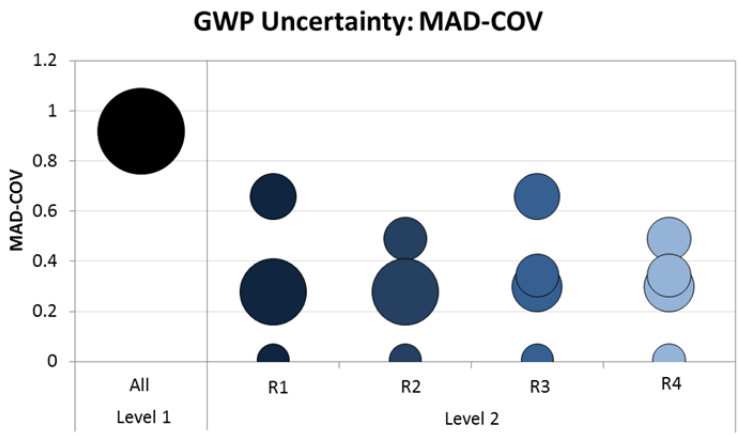
Level 1 includes all polymers database entries, level 2 is based on price, and level 3 is based on the taxonomy described in Figure 3-36.

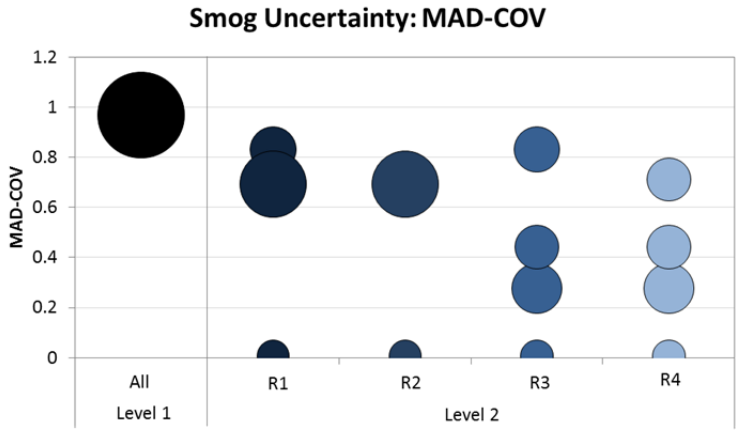


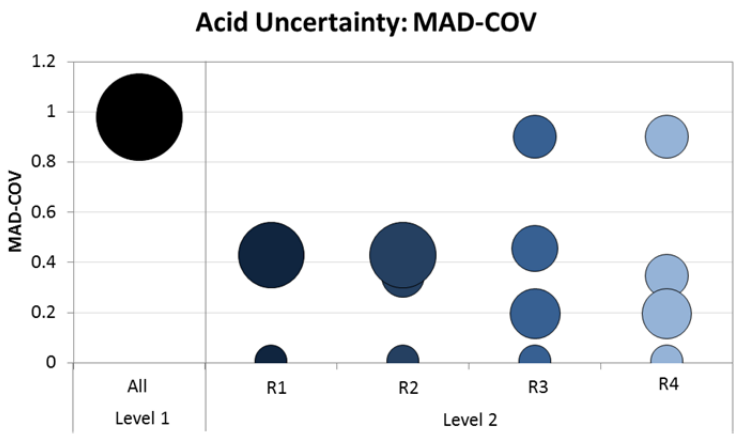
9.3 Precious Metals Taxonomies

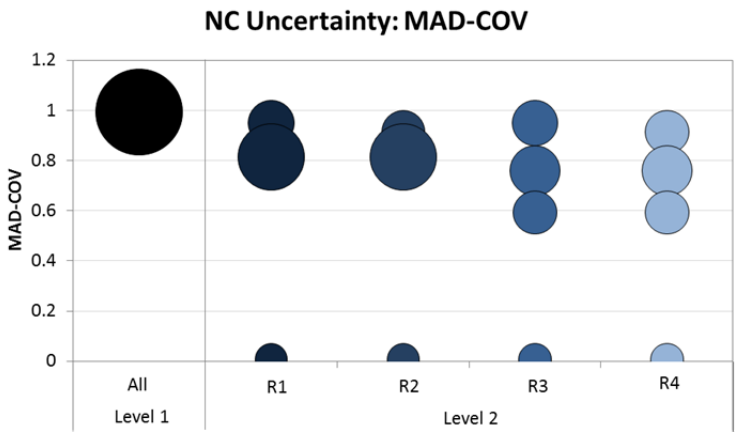
9.3.1 Level 2 Proposed Taxonomies

These plots show the MAD-COVs for the proposed level 2 taxonomies described in Section 3.3.3.






Acid Uncertainty: MAD-COV
MAD-COV
1.2
1
0.8
0.6
0.4
0.2
0
All
Level 1
R1
R2
R3
R4
Level 2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MAD-COV
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1
0.8
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0
All
Level 1
R1
R2
R3
R4
Level 2

10 Appendix C: Taxonomy

LEVEL 1	LEVEL 2	LEVEL 3	LEVEL 4
Metals	P1-A	P1-A-RC<50%	Cadmium sulphide, semiconductor-grade, at plant/US U
Metals	P1-A	P1-A-RC<50%	Cast iron, at plant/RER U
Metals	P1-A	P1-A-RC<50%	DE: BF Steel billet / slab / bloom PE
Metals	P1-A	P1-A-RC<50%	DE: Steel cold rolled coil PE
Metals	P1-A	P1-A-RC<50%	DE: Steel sheet EG PE
Metals	P1-A	P1-A-RC<50%	DE: Steel sheet EG PE
Metals	P1-A	P1-A-RC<50%	DE: Steel sheet EG PE
Metals	P1-A	P1-A-RC<50%	DE: Steel sheet EG PE
Metals	P1-A	P1-A-RC<50%	DE: Steel sheet HDA PE
Metals	P1-A	P1-A-RC<50%	DE: Steel sheet HDA PE
Metals	P1-A	P1-A-RC<50%	DE: Steel sheet HDG PE
Metals	P1-A	P1-A-RC<50%	DE: Steel sheet HDG PE
Metals	P1-A	P1-A-RC<50%	DE: Steel sheet HDG PE
Metals	P1-A	P1-A-RC<50%	DE: Steel sheet HDG PE
Metals	P1-A	P1-A-RC<50%	GLO: Steel cold rolled coil worldsteel
Metals	P1-A	P1-A-RC<50%	GLO: Steel ECCS worldsteel
Metals	P1-A	P1-A-RC<50%	GLO: Steel Electrogalvanized worldsteel
Metals	P1-A	P1-A-RC<50%	GLO: Steel finished cold rolled coil worldsteel
Metals	P1-A	P1-A-RC<50%	GLO: Steel hot dip galvanized worldsteel

LEVEL 1	LEVEL 2	LEVEL 3	LEVEL 4
Metals	P1-A	P1-A-RC<50%	GLO: Steel hot rolled coil worldsteel
Metals	P1-A	P1-A-RC<50%	GLO: Steel organic coated worldsteel
Metals	P1-A	P1-A-RC<50%	GLO: Steel pickled hot rolled coil worldsteel
Metals	P1-A	P1-A-RC<50%	GLO: Steel plate worldsteel
Metals	P1-A	P1-A-RC<50%	GLO: Steel rebar worldsteel
Metals	P1-A	P1-A-RC<50%	GLO: Steel tinplated worldsteel
Metals	P1-A	P1-A-RC<50%	GLO: Steel UO pipe worldsteel
Metals	P1-A	P1-A-RC<50%	GLO: Steel welded pipe worldsteel
Metals	P1-A	P1-A-RC<50%	GLO: Steel wire rod worldsteel
Metals	P1-A	P1-A-RC<50%	Reinforcing steel, at plant/RER U
Metals	P1-A	P1-A-RC<50%	RER: Steel cold rolled coil worldsteel
Metals	P1-A	P1-A-RC<50%	RER: Steel ECCS worldsteel
Metals	P1-A	P1-A-RC<50%	RER: Steel finished cold rolled coil worldsteel
Metals	P1-A	P1-A-RC<50%	RER: Steel hot dip galvanized worldsteel
Metals	P1-A	P1-A-RC<50%	RER: Steel hot rolled coil worldsteel
Metals	P1-A	P1-A-RC<50%	RER: Steel organic coated worldsteel
Metals	P1-A	P1-A-RC<50%	RER: Steel pickled hot rolled coil worldsteel
Metals	P1-A	P1-A-RC<50%	RER: Steel plate worldsteel
Metals	P1-A	P1-A-RC<50%	RER: Steel tinplated worldsteel
Metals	P1-A	P1-A-RC<50%	RER: Steel UO pipe worldsteel

LEVEL 1	LEVEL 2	LEVEL 3	LEVEL 4
Metals	P1-A	P1-A-RC<50%	RER: Steel welded pipe worldsteel
Metals	P1-A	P1-A-RC<50%	Steel, converter, low-alloyed, at plant/RER U
Metals	P1-A	P1-A-RC<50%	Steel, converter, unalloyed, at plant/RER U
Metals	P1-A	P1-A-RC<50%	Steel, low-alloyed, at plant/RER U
Metals	P1-A	P1-A-RC>50%	DE: EAF Steel billet / Slab / Bloom PE
Metals	P1-A	P1-A-RC>50%	DE: Steel billet (100Cr6) PE
Metals	P1-A	P1-A-RC>50%	DE: Steel billet (16MnCr5) PE
Metals	P1-A	P1-A-RC>50%	DE: Steel billet (20MoCr4) PE
Metals	P1-A	P1-A-RC>50%	DE: Steel billet (28Mn6) PE
Metals	P1-A	P1-A-RC>50%	GLO: Steel sections worldsteel
Metals	P1-A	P1-A-RC>50%	RER: Steel sections worldsteel
Metals	P1-A	P1-A-RC>50%	Steel hot rolled coil, blast furnace route, prod. mix, thickness 2-7 mm, width 600-2100 mm RER S
Metals	P1-A	P1-A-RC>50%	Steel hot rolled section, blast furnace and electric arc furnace route, production mix, at plant GLO S
Metals	P1-A	P1-A-RC>50%	Steel rebar, blast furnace and electric arc furnace route, production mix, at plant GLO S
Metals	P1-A	P1-A-RC>50%	Steel, electric, un- and low-alloyed, at plant/RER U
Metals	P1-A	P1-A-Secondary Al	Aluminium, secondary, from new scrap, at plant/RER U
Metals	P1-A	P1-A-Secondary Al	Aluminium, secondary, from old scrap, at plant/RER U
Metals	P1-A	P1-A-Secondary Al	Aluminum, secondary, extruded/RNA
Metals	P1-A	P1-A-Secondary Al	Aluminum, secondary, ingot, at plant/RNA

LEVEL 1	LEVEL 2	LEVEL 3	LEVEL 4
Metals	P1-A	P1-A-Secondary Al	Aluminum, secondary, rolled/RNA
Metals	P1-A	P1-A-Secondary Al	Aluminum, secondary, shape casted/RNA
Metals	P1-B	P1-B-Cu	Copper sheet, technology mix, consumption mix, at plant, 0,6 mm thickness EU-15 S
Metals	P1-B	P1-B-Cu	Copper tube, technology mix, consumption mix, at plant, diameter 15 mm, 1 mm thickness EU-15 S
Metals	P1-B	P1-B-Cu	Copper wire, technology mix, consumption mix, at plant, cross section 1 mm² EU-15 S
Metals	P1-B	P1-B-Cu	Copper, at regional storage/RER U
Metals	P1-B	P1-B-Cu	Copper, from combined metal production, at refinery/SE U
Metals	P1-B	P1-B-Cu	Copper, primary, at refinery/GLO U
Metals	P1-B	P1-B-Cu	Copper, primary, at refinery/ID U
Metals	P1-B	P1-B-Cu	Copper, primary, at refinery/RAS U
Metals	P1-B	P1-B-Cu	Copper, primary, at refinery/RER U
Metals	P1-B	P1-B-Cu	Copper, primary, at refinery/RLA U
Metals	P1-B	P1-B-Cu	Copper, primary, at refinery/RNA U
Metals	P1-B	P1-B-Cu	Copper, primary, couple production nickel/GLO U
Metals	P1-B	P1-B-Cu	Copper, primary, from platinum group metal production/RU U
Metals	P1-B	P1-B-Cu	Copper, primary, from platinum group metal production/ZA U
Metals	P1-B	P1-B-Cu	Copper, secondary, at refinery/RER U
Metals	P1-B	P1-B-Cu	Copper, SX-EW, at refinery/GLO U
Metals	P1-B	P1-B-Cu	DE: Copper mix (99,999% from electrolysis) PE
Metals	P1-B	P1-B-Cu	EU-25: Copper cathode ECI

LEVEL 1	LEVEL 2	LEVEL 3	LEVEL 4
Metals	P1-B	P1-B-Mg	CN: Magnesium PE
Metals	P1-B	P1-B-Mg	Magnesium, at plant/RER U
Metals	P1-B	P1-B-Mg	Magnesium-alloy, AZ91, at plant/RER U
Metals	P1-B	P1-B-Mg	Magnesium-alloy, AZ91, diecasting, at plant/RER U
Metals	P1-B	P1-B-Other	Aluminium alloy, AlMg3, at plant/RER U
Metals	P1-B	P1-B-Other	Aluminium extrusion profile, primary prod., prod. mix, aluminium semi-finished extrusion product RER S
Metals	P1-B	P1-B-Other	Aluminium sheet, primary prod., prod. mix, aluminium semi-finished sheet product RER S
Metals	P1-B	P1-B-Other	Aluminium, primary, at plant/RER U
Metals	P1-B	P1-B-Other	Aluminium, production mix, at plant/RER U
Metals	P1-B	P1-B-Other	Aluminium, production mix, cast alloy, at plant/RER U
Metals	P1-B	P1-B-Other	Aluminium, production mix, wrought alloy, at plant/RER U
Metals	P1-B	P1-B-Other	Aluminum ingot, production mix, at plant/US
Metals	P1-B	P1-B-Other	Aluminum, primary, ingot, at plant/RNA
Metals	P1-B	P1-B-Other	Antimony, at refinery/CN U
Metals	P1-B	P1-B-Other	Brass, at plant/CH U
Metals	P1-B	P1-B-Other	Brazing solder, cadmium free, at plant/RER U
Metals	P1-B	P1-B-Other	Bronze, at plant/CH U
Metals	P1-B	P1-B-Other	Cadmium, primary, at plant/GLO U
Metals	P1-B	P1-B-Other	Cadmium, semiconductor-grade, at plant/US U
Metals	P1-B	P1-B-Other	Chromium steel 18/8, at plant/RER U

LEVEL 1	LEVEL 2	LEVEL 3	LEVEL 4
Metals	P1-B	P1-B-Other	DE: Aluminium extrusion profile mix PE
Metals	P1-B	P1-B-Other	DE: Aluminium ingot mix PE
Metals	P1-B	P1-B-Other	DE: Aluminium sheet mix PE
Metals	P1-B	P1-B-Other	DE: Lead (99,995%) PE
Metals	P1-B	P1-B-Other	DE: Lead PE
Metals	P1-B	P1-B-Other	DE: Zinc redistilled mix PE
Metals	P1-B	P1-B-Other	Lead, at regional storage/RER U
Metals	P1-B	P1-B-Other	Lead, from combined metal production, at refinery/SE U
Metals	P1-B	P1-B-Other	Lead, primary, at plant/GLO U
Metals	P1-B	P1-B-Other	Lead, primary, consumption mix, at plant DE S
Metals	P1-B	P1-B-Other	Lead, secondary, at plant/RER U
Metals	P1-B	P1-B-Other	Manganese, at regional storage/RER U
Metals	P1-B	P1-B-Other	RER: Aluminium extrusion profile PE
Metals	P1-B	P1-B-Other	RER: Aluminium foil PE
Metals	P1-B	P1-B-Other	RER: Aluminium ingot mix PE
Metals	P1-B	P1-B-Other	RER: Aluminium profile PE
Metals	P1-B	P1-B-Other	RER: Aluminium sheet EAA
Metals	P1-B	P1-B-Other	RER: Aluminium sheet mix PE
Metals	P1-B	P1-B-Other	RER: Aluminum ingot mix (2005) EAA
Metals	P1-B	P1-B-Other	RER: Brass (CuZn20) PE

LEVEL 1	LEVEL 2	LEVEL 3	LEVEL 4
Metals	P1-B	P1-B-Other	RER: Brass (CuZn39Pb3) PE
Metals	P1-B	P1-B-Other	RER: Red brass PE
Metals	P1-B	P1-B-Other	RER: Stainless steel cold rolled coil (304) Eurofer
Metals	P1-B	P1-B-Other	RER: Stainless steel cold rolled coil (316) Eurofer
Metals	P1-B	P1-B-Other	RER: Stainless steel cold rolled coil (430) Eurofer
Metals	P1-B	P1-B-Other	RER: Stainless steel Quarto plate (2205) Eurofer
Metals	P1-B	P1-B-Other	RER: Stainless steel Quarto plate (304) Eurofer
Metals	P1-B	P1-B-Other	RER: Stainless steel Quarto plate (316) Eurofer
Metals	P1-B	P1-B-Other	RER: Stainless steel white hot rolled coil (304) Eurofer
Metals	P1-B	P1-B-Other	RER: Stainless steel white hot rolled coil (316) Eurofer
Metals	P1-B	P1-B-Other	RER: Stainless steel white hot rolled coil (430) Eurofer
Metals	P1-B	P1-B-Other	Special high grade zinc, primary production, production mix, at plant GLO S
Metals	P1-B	P1-B-Other	Steel, converter, chromium steel 18/8, at plant/RER U
Metals	P1-B	P1-B-Other	Steel, electric, chromium steel 18/8, at plant/RER U
Metals	P1-B	P1-B-Other	Titanium zinc plate, without pre-weathering, at plant/DE U
Metals	P1-B	P1-B-Other	Zinc, from combined metal production, at refinery/SE U
Metals	P1-B	P1-B-Other	Zinc, primary, at regional storage/RER U
Metals	P1-B	P1-B-Other	Zinc, sheet/GLO
Metals	P1-B	P1-B-Other	Zinc, special high grade/GLO
Metals	P1-C	P1-C-Ga	Gallium, semiconductor-grade, at plant/GLO U

LEVEL 1	LEVEL 2	LEVEL 3	LEVEL 4
Metals	P1-C	P1-C-Ga	Gallium, semiconductor-grade, at regional storage/RER U
Metals	P1-C	P1-C-In	Indium, at regional storage/RER U
Metals	P1-C	P1-C-Other	Cadmium chloride, semiconductor-grade, at plant/US U
Metals	P1-C	P1-C-Other	Cadmium telluride, semiconductor-grade, at plant/US U
Metals	P1-C	P1-C-Other	Chromium, at regional storage/RER U
Metals	P1-C	P1-C-Other	Cobalt, at plant/GLO U
Metals	P1-C	P1-C-Other	Copper telluride cement, from copper production/GLO U
Metals	P1-C	P1-C-Other	CZ single crystalline silicon, electronics, at plant/RER U
Metals	P1-C	P1-C-Other	CZ single crystalline silicon, photovoltaics, at plant/RER U
Metals	P1-C	P1-C-Other	GLO: Silicon mix (99%) PE
Metals	P1-C	P1-C-Other	Iron-nickel-chromium alloy, at plant/RER U
Metals	P1-C	P1-C-Other	Lithium, at plant/GLO U
Metals	P1-C	P1-C-Other	Molybdenum, at regional storage/RER U
Metals	P1-C	P1-C-Other	Nickel, 99.5%, at plant/GLO U
Metals	P1-C	P1-C-Other	Nickel, primary, from platinum group metal production/ZA U
Metals	P1-C	P1-C-Other	Silicon, electronic grade, at plant/DE U
Metals	P1-C	P1-C-Other	Silicon, electronic grade, off-grade, at plant/DE U
Metals	P1-C	P1-C-Other	Silicon, multi-Si, casted, at plant/RER U
Metals	P1-C	P1-C-Other	Silicon, production mix, photovoltaics, at plant/GLO U
Metals	P1-C	P1-C-Other	Silicon, solar grade, modified Siemens process, at plant/RER U

LEVEL 1	LEVEL 2	LEVEL 3	LEVEL 4
Metals	P1-C	P1-C-Other	Soft solder, Sn97Cu3, at plant/RER U
Metals	P1-C	P1-C-Other	Solder, bar, Sn63Pb37, for electronics industry, at plant/GLO U
Metals	P1-C	P1-C-Other	Solder, bar, Sn95.5Ag3.9Cu0.6, for electronics industry, at plant/GLO U
Metals	P1-C	P1-C-Other	Solder, paste, Sn63Pb37, for electronics industry, at plant/GLO U
Metals	P1-C	P1-C-Other	Solder, paste, Sn95.5Ag3.9Cu0.6, for electronics industry, at plant/GLO U
Metals	P1-C	P1-C-Other	Tellurium, semiconductor-grade, at plant/GLO U
Metals	P1-C	P1-C-Other	Tin, at regional storage/RER U
Metals	P1-C	P1-C-Ta	Tantalum, powder, capacitor-grade, at regional storage/GLO U
Metals	P1-Mercury	P1-Mercury	Mercury, liquid, at plant/GLO U
Metals	P1-Nickel Outlier	P1-Nickel Outlier	Nickel, primary, from platinum group metal production/RU U
Polymers	Price-A	Price-A	Acrylic binder, 34% in H2O, at plant/RER U
Polymers	Price-A	Price-A	Acrylic dispersion, 65% in H2O, at plant/RER U
Polymers	Price-A	Price-A	Alkyd resin, long oil, 70% in white spirit, at plant/RER U
Polymers	Price-A	Price-A	Anionic resin, at plant/CH U
Polymers	Price-A	Price-A	Carboxymethyl cellulose, powder, at plant/RER S
Polymers	Price-A	Price-A	Cationic resin, at plant/CH U
Polymers	Price-A	Price-A	DE: Polyester Resin unsaturated (UP) PE
Polymers	Price-A	Price-A	DE: Polyethylene High Density Granulate (PE-HD) Mix PE
Polymers	Price-A	Price-A	DE: Polyethylene Terephthalate Granulate (PET) via DMT PE
Polymers	Price-A	Price-A	DE: Polymethylmethacrylate granulate (PMMA) PE

LEVEL 1	LEVEL 2	LEVEL 3	LEVEL 4
Polymers	Price-A	Price-A	DE: Polypropylene granulate (PP) mix PE
Polymers	Price-A	Price-A	DE: Polystyrene granulate (PS) mix PE
Polymers	Price-A	Price-A	DE: Polyvinyl Chloride Granulate (Suspension; S-PVC) Mix PE
Polymers	Price-A	Price-A	DE: Styrene-Butadiene Rubber (SBR) Mix PE
Polymers	Price-A	Price-A	Ethylene vinyl acetate copolymer, at plant/RER U
Polymers	Price-A	Price-A	Ethylvinylacetate, foil, at plant/RER U
Polymers	Price-A	Price-A	EU-27: Polyacrylonitrile Fibres (PAN) PE
Polymers	Price-A	Price-A	EU-27: Polyethylene terephthalate fibres (PET) PE
Polymers	Price-A	Price-A	EU-27: Polypropylene fibers (PP) PE
Polymers	Price-A	Price-A	Fleece, polyethylene, at plant/RER U
Polymers	Price-A	Price-A	General purpose polystyrene, at plant/RNA
Polymers	Price-A	Price-A	HDPE bottles E
Polymers	Price-A	Price-A	HDPE pipes E
Polymers	Price-A	Price-A	High density polyethylene resin, at plant/RNA
Polymers	Price-A	Price-A	Latex, at plant/RER S
Polymers	Price-A	Price-A	LDPE bottles E
Polymers	Price-A	Price-A	LDPE ETH S
Polymers	Price-A	Price-A	Linear low density polyethylene resin, at plant/RNA
Polymers	Price-A	Price-A	Low density polyethylene resin, at plant/RNA
Polymers	Price-A	Price-A	Melamine formaldehyde resin, at plant/RER U

LEVEL 1	LEVEL 2	LEVEL 3	LEVEL 4
Polymers	Price-A	Price-A	Melamine-urea-formaldehyde hardener, at plant/US
Polymers	Price-A	Price-A	Melamine-urea-formaldehyde resin, at plant/US
Polymers	Price-A	Price-A	Oriented polypropylene film E
Polymers	Price-A	Price-A	Packaging film, LDPE, at plant/RER U
Polymers	Price-A	Price-A	PET (amorphous) E
Polymers	Price-A	Price-A	PET (bottle grade) E
Polymers	Price-A	Price-A	PET bottles E
Polymers	Price-A	Price-A	PET film (production only) E
Polymers	Price-A	Price-A	Phenol formaldehyde, at plant/US
Polymers	Price-A	Price-A	Phenolic resin, at plant/RER U
Polymers	Price-A	Price-A	Phenol-resorcinol-formaldehyde hardener, at plant/US
Polymers	Price-A	Price-A	Polybutadiene granulate (PB), production mix, at plant RER
Polymers	Price-A	Price-A	Polybutadiene, at plant/RER U
Polymers	Price-A	Price-A	Polybutadiene, at plant/RNA
Polymers	Price-A	Price-A	Polyester resin, unsaturated, at plant/RER U
Polymers	Price-A	Price-A	Polyethylene high density granulate (PE-HD), production mix, at plant RER
Polymers	Price-A	Price-A	Polyethylene low density granulate (PE-LD), production mix, at plant RER
Polymers	Price-A	Price-A	Polyethylene low linear density granulate (PE-LLD), production mix, at plant RER
Polymers	Price-A	Price-A	Polyethylene terephthalate (PET) granulate, production mix, at plant, amorphous RER
Polymers	Price-A	Price-A	Polyethylene terephthalate (PET) granulate, production mix, at plant, bottle grade RER

LEVEL 1	LEVEL 2	LEVEL 3	LEVEL 4
Polymers	Price-A	Price-A	Polyethylene terephthalate fibres (PET), via dimethyl terephthalate (DMT), prod. mix, EU-27 S
Polymers	Price-A	Price-A	Polyethylene terephthalate resin, at plant/kg/RNA
Polymers	Price-A	Price-A	Polyethylene terephthalate, granulate, amorphous, at plant/RER U
Polymers	Price-A	Price-A	Polyethylene terephthalate, granulate, bottle grade, at plant/RER U
Polymers	Price-A	Price-A	Polyethylene, HDPE, granulate, at plant/RER U
Polymers	Price-A	Price-A	Polyethylene, LDPE, granulate, at plant/RER U
Polymers	Price-A	Price-A	Polyethylene, LLDPE, granulate, at plant/RER U
Polymers	Price-A	Price-A	Polylactide, granulate, at plant/GLO U
Polymers	Price-A	Price-A	Polymethyl methacrylate (PMMA) beads, production mix, at plant RER
Polymers	Price-A	Price-A	Polymethyl methacrylate, beads, at plant/RER U
Polymers	Price-A	Price-A	Polymethyl methacrylate, sheet, at plant/RER U
Polymers	Price-A	Price-A	Polypropylene fibres (PP), crude oil based, production mix, at plant, PP granulate without additives EU-27 S
Polymers	Price-A	Price-A	Polypropylene granulate (PP), production mix, at plant RER
Polymers	Price-A	Price-A	Polypropylene injection moulding E
Polymers	Price-A	Price-A	Polypropylene resin, at plant/RNA
Polymers	Price-A	Price-A	Polypropylene, granulate, at plant/RER U
Polymers	Price-A	Price-A	Polystyrene (general purpose) granulate (GPPS), prod. mix, RER
Polymers	Price-A	Price-A	Polystyrene expandable granulate (EPS), production mix, at plant RER
Polymers	Price-A	Price-A	Polystyrene thermoforming E

LEVEL 1	LEVEL 2	LEVEL 3	LEVEL 4
Polymers	Price-A	Price-A	Polystyrene, expandable, at plant/RER U
Polymers	Price-A	Price-A	Polystyrene, general purpose, GPPS, at plant/RER U
Polymers	Price-A	Price-A	Polyvinyl chloride resin, at plant/RNA
Polymers	Price-A	Price-A	Polyvinylchloride resin (B-PVC), bulk polymerisation, production mix, at plant RER
Polymers	Price-A	Price-A	Polyvinylchloride resin (E-PVC), emulsion polymerisation, production mix, at plant RER
Polymers	Price-A	Price-A	Polyvinylchloride resin (S-PVC), suspension polymerisation, production mix, at plant RER
Polymers	Price-A	Price-A	Polyvinylchloride, at regional storage/RER U
Polymers	Price-A	Price-A	Polyvinylchloride, bulk polymerised, at plant/RER U
Polymers	Price-A	Price-A	Polyvinylchloride, emulsion polymerised, at plant/RER U
Polymers	Price-A	Price-A	Polyvinylchloride, suspension polymerised, at plant/RER U
Polymers	Price-A	Price-A	PVC (bulk polymerisation) E
Polymers	Price-A	Price-A	PVC (emulsion polyerisation) E
Polymers	Price-A	Price-A	PVC (suspension polymerisation) E
Polymers	Price-A	Price-A	PVC calendered sheet E
Polymers	Price-A	Price-A	PVC film E
Polymers	Price-A	Price-A	PVC injection moulding E
Polymers	Price-A	Price-A	PVC pipe E
Polymers	Price-A	Price-A	Recycled postconsumer HDPE pellet/RNA
Polymers	Price-A	Price-A	Recycled postconsumer PET flake/RNA
Polymers	Price-A	Price-A	Recycled postconsumer PET pellet/RNA

LEVEL 1	LEVEL 2	LEVEL 3	LEVEL 4
Polymers	Price-A	Price-A	RER: Polyethylene film (PE-LD) PlasticsEurope
Polymers	Price-A	Price-A	Resin size, at plant/RER U
Polymers	Price-A	Price-A	Styrene-acrylonitrile copolymer (SAN) E
Polymers	Price-A	Price-A	Styrene-acrylonitrile copolymer, SAN, at plant/RER U
Polymers	Price-A	Price-A	Urea formaldehyde resin, at plant/RER U
Polymers	Price-B	Price-B-Epoxy	Epoxy resin insulator (Al2O3), at plant/RER U
Polymers	Price-B	Price-B-Epoxy	Epoxy resin insulator (SiO2), at plant/RER U
Polymers	Price-B	Price-B-Epoxy	Epoxy resin, liquid, at plant/RER U
Polymers	Price-B	Price-B-Epoxy	Epoxy resin, liquid, disaggregated data, at plant/RER U
Polymers	Price-B	Price-B-Epoxy	Liquid epoxy resins E
Polymers	Price-B	Price-B-Nylon	EU-27: Polyamide 6.6 fibres (PA 6.6) PE
Polymers	Price-B	Price-B-Nylon	Glass fibre reinforced plastic, polyamide, injection moulding, at plant/RER U
Polymers	Price-B	Price-B-Nylon	Nylon 6 glass filled (PA 6 GF), production mix, at plant RER
Polymers	Price-B	Price-B-Nylon	Nylon 6 granulate (PA 6), production mix, at plant RER
Polymers	Price-B	Price-B-Nylon	Nylon 6, at plant/RER U
Polymers	Price-B	Price-B-Nylon	Nylon 6, glass-filled, at plant/RER U
Polymers	Price-B	Price-B-Nylon	Nylon 66 GF 30 compound (PA 66 GF 30), production mix, at plant RER
Polymers	Price-B	Price-B-Nylon	Nylon 66 granulate (PA 66), production mix, at plant RER
Polymers	Price-B	Price-B-Nylon	Nylon 66, at plant/RER U
Polymers	Price-B	Price-B-Nylon	Nylon 66, glass-filled, at plant/RER U

LEVEL 1	LEVEL 2	LEVEL 3	LEVEL 4
Polymers	Price-B	Price-B-Nylon	Polyamide 6.6 fibres (PA 6.6), from adipic acid and hexamethylene diamine (HMDA), prod. mix, EU-27 S
Polymers	Price-B	Price-B-Other	Acrylonitrile-butadiene-styrene copolymer resin, at plant/RNA
Polymers	Price-B	Price-B-Other	Acrylonitrile-butadiene-styrene copolymer, ABS, at plant/RER U
Polymers	Price-B	Price-B-Other	Acrylonitrile-butadiene-styrene granulate (ABS), production mix, at plant RER
Polymers	Price-B	Price-B-Other	DE: Acrylonitrile-Butadiene-Styrene Granulate (ABS) Mix PE
Polymers	Price-B	Price-B-Other	DE: Polycarbonate Granulate (PC) PE
Polymers	Price-B	Price-B-Other	DE: Polypropylene / Ethylene Propylene Diene Elastomer Granulate (PP/EPDM) Mix PE
Polymers	Price-B	Price-B-Other	DE: Polypropylene GMT part PE
Polymers	Price-B	Price-B-Other	DE: Polystyrene High Impact Granulate (HI-PS) Mix PE
Polymers	Price-B	Price-B-Other	DE: Sheet Moulding Compound resin mat (SMC) PE
Polymers	Price-B	Price-B-Other	EU-25: Polycarbonate granulate (PC) PlasticsEurope
Polymers	Price-B	Price-B-Other	Glass fibre reinforced plastic, polyester resin, hand lay-up, at plant/RER U
Polymers	Price-B	Price-B-Other	High impact polystyrene granulate (HIPS), production mix, at plant RER
Polymers	Price-B	Price-B-Other	High impact polystyrene resin, at plant/RNA
Polymers	Price-B	Price-B-Other	Modified starch, at plant/RER U
Polymers	Price-B	Price-B-Other	Polycarbonate granulate (PC), production mix, at plant RER
Polymers	Price-B	Price-B-Other	Polycarbonate, at plant/RER U
Polymers	Price-B	Price-B-Other	Polystyrene, high impact, HIPS, at plant/RER U
Polymers	Price-B	Price-B-Other	Polyurethane flexible foam E
Polymers	Price-B	Price-B-Other	Polyurethane rigid foam E

LEVEL 1	LEVEL 2	LEVEL 3	LEVEL 4
Polymers	Price-B	Price-B-Other	Polyurethane, flexible foam, at plant/RER U
Polymers	Price-B	Price-B-Other	Polyurethane, rigid foam, at plant/RER U
Polymers	Price-B	Price-B-Other	Polyvinylidenchloride, granulate, at plant/RER U
Polymers	Price-B	Price-B-Other	RER: Polyisocyanurate (PIR high-density foam) PE
Polymers	Price-B	Price-B-Other	Soy-based resin, at plant/RNA
Polymers	Price-B	Price-B-Other	Synthetic rubber, at plant/RER U
Polymers	Price-C	Price-C-PPS	Polyphenylene sulfide, at plant/GLO U
Polymers	Price-C	Price-C-PVF	Polyvinylfluoride film, at plant/US U
Polymers	Price-C	Price-C-PVF	Polyvinylfluoride, at plant/US U
Polymers	Price-C	Price-C-PVF	Polyvinylfluoride, dispersion, at plant/US U
Polymers	Price-PTFE	Price-PTFE	Tetrafluoroethylene film, on glass/RER U
Polymers	Price-PTFE	Price-PTFE	Tetrafluoroethylene, at plant/RER U
Polymers	Price-PRF Outlier	Price-PRF Outlier	Phenol-resorcinol-formaldehyde resin, at plant/US
Precious Metals	R4-Ag	R4-Ag	Silver, at regional storage/RER U
Precious Metals	R4-Ag	R4-Ag	Silver, from combined gold-silver production, at refinery/CL U
Precious Metals	R4-Ag	R4-Ag	Silver, from combined gold-silver production, at refinery/GLO U
Precious Metals	R4-Ag	R4-Ag	Silver, from combined gold-silver production, at refinery/PE U
Precious Metals	R4-Ag	R4-Ag	Silver, from combined gold-silver production, at refinery/PG U
Precious Metals	R4-Ag	R4-Ag	Silver, from combined metal production, at beneficiation/SE U
Precious Metals	R4-Ag	R4-Ag	Silver, from combined metal production, at refinery/SE U

LEVEL 1	LEVEL 2	LEVEL 3	LEVEL 4
Precious Metals	R4-Ag	R4-Ag	Silver, from copper production, at refinery/GLO U
Precious Metals	R4-Ag	R4-Ag	Silver, from lead production, at refinery/GLO U
Precious Metals	R4-Au	R4-Au	Gold, at refinery/AU U
Precious Metals	R4-Au	R4-Au	Gold, at refinery/CA U
Precious Metals	R4-Au	R4-Au	Gold, at refinery/TZ U
Precious Metals	R4-Au	R4-Au	Gold, at refinery/US U
Precious Metals	R4-Au	R4-Au	Gold, at refinery/ZA U
Precious Metals	R4-Au	R4-Au	Gold, at regional storage/RER U
Precious Metals	R4-Au	R4-Au	Gold, from combined gold-silver production, at refinery/CL U
Precious Metals	R4-Au	R4-Au	Gold, from combined gold-silver production, at refinery/PE U
Precious Metals	R4-Au	R4-Au	Gold, from combined gold-silver production, at refinery/PG U
Precious Metals	R4-Au	R4-Au	Gold, from combined metal production, at beneficiation/SE U
Precious Metals	R4-Au	R4-Au	Gold, from combined metal production, at refinery/SE U
Precious Metals	R4-Au	R4-Au	Gold, primary, at refinery/GLO U
Precious Metals	R4-PGM	R4-PGM	Palladium, at regional storage/RER U
Precious Metals	R4-PGM	R4-PGM	Palladium, primary, at refinery/RU U
Precious Metals	R4-PGM	R4-PGM	Palladium, primary, at refinery/ZA U
Precious Metals	R4-PGM	R4-PGM	Platinum, at regional storage/RER U
Precious Metals	R4-PGM	R4-PGM	Platinum, primary, at refinery/RU U
Precious Metals	R4-PGM	R4-PGM	Platinum, primary, at refinery/ZA U

LEVEL 1	LEVEL 2	LEVEL 3	LEVEL 4
Precious Metals	R4-PGM	R4-PGM	Rhodium, at regional storage/RER U
Precious Metals	R4-PGM	R4-PGM	Rhodium, primary, at refinery/RU U
Precious Metals	R4-PGM	R4-PGM	Rhodium, primary, at refinery/ZA U
Precious Metals	R4-Secondary Ag	R4-Secondary Ag	Silver, secondary, at precious metal refinery/SE U
Precious Metals	R4-Secondary Au/PGM	R4-Secondary Au/PGM	Gold, secondary, at precious metal refinery/SE U
Precious Metals	R4-Secondary Au/PGM	R4-Secondary Au/PGM	Palladium, secondary, at precious metal refinery/SE U
Precious Metals	R4-Secondary Au/PGM	R4-Secondary Au/PGM	Palladium, secondary, at refinery/RER U
Precious Metals	R4-Secondary Au/PGM	R4-Secondary Au/PGM	Platinum, secondary, at refinery/RER U
Precious Metals	R4-Secondary Au/PGM	R4-Secondary Au/PGM	Rhodium, secondary, at refinery/RER U