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Design for Recycling: Evaluation and Efficient Alloy Modification

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Abstract

As design for recycling becomes more broadly applied in material and product design, analytical tools to quantify the environmental implications of design choices will become a necessity. Currently, few systematic methods exist to measure and direct the metallurgical alloy design process in regards to recyclability. This is due, in part, to the difficulty in evaluating such a context-dependent property as recyclability of an alloy, which will depend on the types of scraps available to producers, the compositional characteristics of those scraps, their yield, and the alloy itself. This paper presents a chance-constrained based optimization method that explores the effects of strategic alloy choice in aluminum production on the ability to utilize secondary materials in the alloy's raw material portfolio. Two cases are presented to demonstrate the model's ability to both directly evaluate the recyclability of specific alloy formulations and proactively identify the most effective alloy modification strategies that can drive increased recycling.

1.0 Introduction

One of the key engineering challenges of the 21st century will be reducing the harmful effects associated with a growing population and the attendant flows of materials[1, 2]. The materials community is uniquely positioned to play a central role in addressing these problems by fundamentally changing the materials and processes used by society. For this to happen, materials experts must begin to consider the environmental impacts of their design choices and will require additional analytical tools to quantify those broader implications. This paper begins to address this need for at least one element of a material's environmental performance -- recyclability.

1.1 Metals Recycling: A Case of Aluminum

It is well known for many materials, and particularly for metals, that substitution of primary with secondary resources, i.e. those recovered from manufacturing waste or end-of-life products, decreases energy consumption and the attendant environmental burden (Figure 1). Aluminum, the material selected as a case for this document serves as an excellent example due to the large energy differences between primary and secondary production: 175 MJ/kg for primary compared to 10-20 MJ/kg for secondary[3].

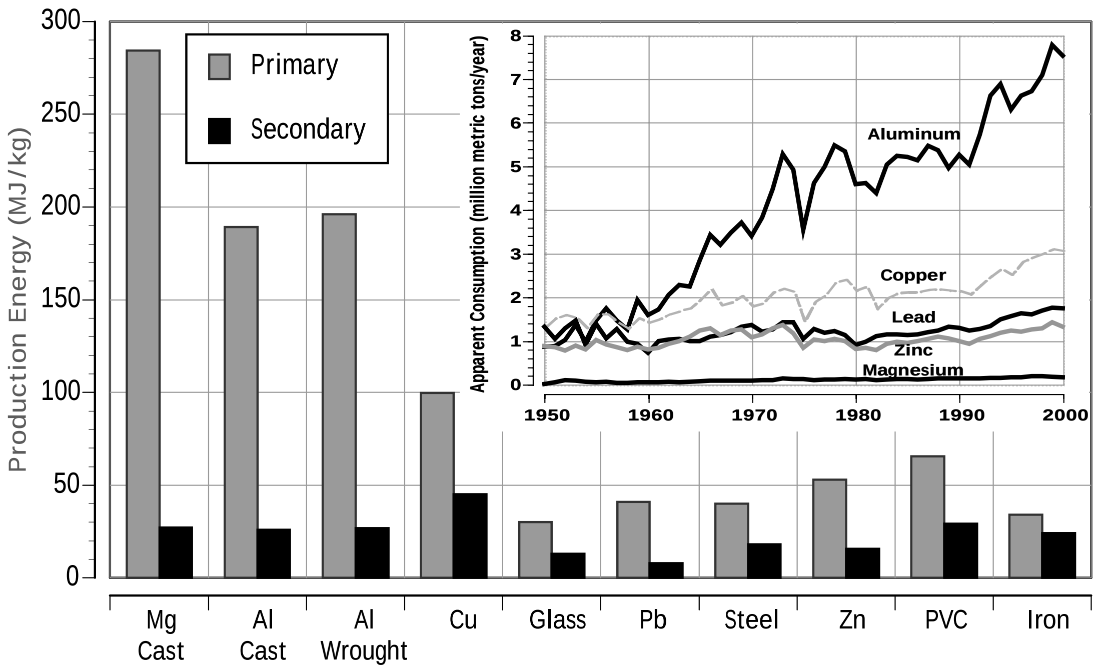

Figure 1. Primary and secondary energy usage for various materials[3]; inset, US consumption of various metals[4].

Fortunately, this self-same energy advantage creates a strong economic incentive to recycle. This benefit is manifest in the rapid growth in secondary aluminum production (Figure 2)[4, 5], which is far outpacing growth in primary production. To date, secondary production has focused on satisfying demand for compositionally forgiving cast alloys and the carefully designed alloy systems used for can stock. If secondary production is to sustain its growth trend, the sinks for secondary material will also need to expand. In fact, several authors have specifically commented on the pending limits of the traditional sinks 380, 3105, and 3004/3104[6, 7].

Fortunately, several technological strategies are possible to address this need. These include more effective scrap upgrading (sorting or compositional modification), improved recycling operational practices, informed alloy selection, and/or targeted alloy design. To guide metals technology development in any of these directions, it is necessary for the metallurgist to be able to evaluate the implications on recyclability. This paper explores the use of a modeling framework to perform such an evaluation and demonstrates its application to guiding one of these strategies – alloy design[1].

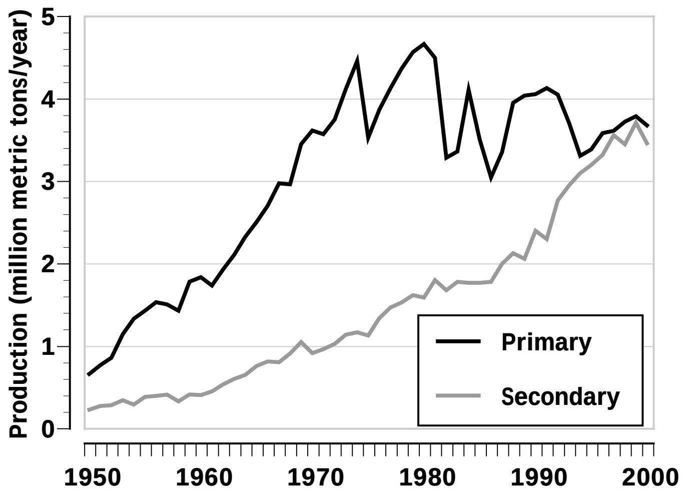

Figure 2. Primary and secondary production of aluminum in the United States; in recent years, secondary production has outpaced the growth of primary production substantially

1.2 The Question of Recycling Friendly Alloy Design

How to make alloys more recycling friendly or, in other words, more able to accommodate scrap materials in their production portfolios, is a challenging question. Industry experts and literature have provided a variety of suggestions including higher maximum compositional specifications for certain elements that will not adversely affect alloy properties, wider specification targets (i.e. higher maximums and lower minimums), or translating compositional constraints to specifications based on performance[7]. Other suggestions involve modifying the forming and joining of aluminum, for example, replacing conventional welding with mechanical joining, laser welding, or friction stir welding[8]. Some even propose legislation or regulations to limit the number of alloys that can be used in certain products such as cars or aircraft[9]. However, no quantitative assessments of the efficacy of these suggestions on the ability of a recycler or recycling system to use more secondary raw materials have been performed. Furthermore, no methodology has been discussed that would quantitatively assess where and to what extent these strategies should be applied.

Despite these specific issues, a range of literature has examined the use of decision-analysis models to improve the economic and resource use performance of recycling operations. The most pertinent

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[1] The focus herein on alloy design is not meant to imply that this is the most critical strategy. In fact, the most economically efficient path to improving the recycling effectiveness of any materials system will likely involve combinations of all four strategies. Nevertheless, evaluating which or which combination of strategies are preferred can only be possible once the potential and impact of each has been fully characterized. This work provides a step toward that goal.

include those that apply a range of mathematical programming techniques to improve decisions about raw materials purchasing strategy , technology selection[10-12], and the application of upgrading and sorting for secondary raw materials[13, 14]. Although notionally these models can be used iteratively to evaluate how some change would affect the ability to use secondary raw materials, none are capable of evaluating the design of multi-specification alloys.

The primary challenge of evaluating alloy recycling-friendliness is that it is a context dependent property; how much scrap an alloy can accommodate will be based on not only the compositional characteristics of the alloy itself, but also the types of scraps available to producers, the compositional characteristics of those scraps, and their metallic yield. As a result, a method to evaluate recyclability must be able to account for the confluence of these detailed effects.

Two sets of previous work on decision-analysis models have been specifically applied to recycling performance of secondary aluminum production and form the basis for addressing this need. The first set of studies by Reuter, van Schaik, and others[10-13, 15-17] utilized dynamic modeling and extensive product data to optimize the recycling of end-of-life vehicles, including the light-metals within them. This work and the models it presents can be used to guide operational and technological decisions by recyclers and to provide reasonable recovery expectations for recyclers, and more broadly, legislators. The second set is previous work by the authors [18] that described schematic, compositionally-specific mathematical programming models that identify the optimal raw materials mix to blend to produce a given alloy production portfolio. These models were used to evaluate the effectiveness of alloy substitution and improved operational practices to increase potential scrap use. In this work, the authors hypothesized that model-derived sensitivity analysis information could be used to direct alloy design and demonstrated that, for a stylized case, such sensitivity analysis information varied significantly across specification and alloy.

This paper extends this previous work by demonstrating systematically how such decision-support models can be used to (1) directly evaluate the potential scrap usage of alloys across a range of raw materials contexts and (2) proactively identify the most effective alloy modification strategies that can drive increased potential scrap use. With regard to the latter, this paper extends previous discussions by exploring in detail how sensitivity analysis information actually correlates with potential scrap use performance and how both the sensitivity analysis information and the associated potential scrap use effect changes with individual and coordinated specification modifications. In exploring the latter for two distinct cases, this paper suggests that real potential exists for increasing potential scrap use through alloy redesign while remaining within established compositional specifications. Finally, this paper extends previous work in this space by presenting a schematic algorithm for explicitly incorporating uncertain metal yield into the analyses of alloy design specifically, and recycler operational decisions more broadly.

Both the model and cases discussed herein are intended to be schematic in nature. Much work still remains to capture the metallurgical complexity of the recycling process; nevertheless, the results presented show that this framework holds promise to be a valuable tool in the metallurgists toolkit. Such a tool would always be but a single element in the overall alloy design process. Traditional and emerging metallurgical methods will always be required to identify alloys capable of meeting demanding physical performance requirements. Nevertheless, efficient design of resource-conscious materials depends upon analytical tools capable of projecting the impact of design choices on recycling performance.

2.0 Methods

2.1 Evaluating Recyclability: Optimization Modeling/Linear Programming

Modeling tools that make use of linear optimization techniques are broadly available to support the decision-making of metallurgical production planners [19, 20] The primary results of such an optimization model are a set of decision variables that will yield the optimal objective function. In the case of batch planning tools for secondary alloy production, these decision variables are the amounts of scrap and primary raw materials that can be used to produce the targeted alloys. Later in this paper, such results will be used directly to evaluate the recyclability of specific proposed alloy formulations.

Additionally, linear optimization models provide a powerful set of results that quantify the sensitivity of the optimal result to changes in assumptions. Among these sensitivity parameters are what is known as “shadow prices”. A shadow price is defined for each binding constraint in the optimization problem and its value is the change in the objective function at the optimum for a unit change in that constraint[14] as expressed in Equation (1.1). Each shadow price has a range of validity associated with it.

$$SP_{\text{Constraint}} = \frac{\delta(\text{Production Cost})}{\delta(\text{Constraint})} \quad (1.1)$$

For the model presented subsequently, there are three potential classes of shadow prices that are reported. These are shadow prices for 1) constraints on availability, 2) constraints on demand, and 3) constraints on composition. The latter will be used to provide quantitative guidance to the design of alloys with improved recyclability. Interested readers should consult[14] for a lengthier discussion on the value of the other shadow price analyses for strategic decision-making around secondary materials.

2.2 Model Formulation

The first step to improving the recycling performance of specific alloys is a model capable of evaluating their potential for secondary raw materials use across a range of production contexts. To accomplish this, this paper will explore the use of a modified formulation of a schematic model initially described in [14]. Specifically, the model examines the problem of mixing arbitrary quantities of raw materials (pure or scrap aluminum) to produce a set of new aluminum alloys under certain constraints (e.g., the mixing of raw materials must meet compositional specifications for final products). The goal of this model is to identify a production plan that will minimize the overall expected production costs (cf. Equation (1.2)) while meeting finished good compositional specifications. Generally, this exactly matches at least one set of decisions faced by a cast house manager. Compared to prevalent batch mixing tools used in cast houses today, the model formulation presented herein differs primarily in that it optimizes raw material use across the production of an entire portfolio of alloys simultaneously and that it allows for key operational uncertainties to be explicitly considered in the evaluation process. It differs substantively from the presentation in [17, 21] in that it comprehends the effects of imperfect metallurgical yield and that it allows for that yield to be represented as an uncertain stochastic parameter.

A model that is capable of treating composition and yield as uncertain parameters was specifically selected for three key reasons. First of all, assessments that treat uncertainty implicitly, generally based on mean expected conditions, assume that deviation from that value has symmetric consequences. For many production related decisions within the cast-house, the repercussion of missing a forecast are inherently non-symmetrical. Secondly, deterministic approaches generally do not provide proactive mechanisms to modify production strategies as prevailing conditions evolve. Finally, previous work by the authors has shown that treating uncertainty explicitly in evaluating recycler operational decisions suggests strategies that improve economics and scrap use potential.

The core model, as presented in can be formulated as follows in Equations (1.2) through (1.6). As stated above, the goal of this model is to identify the production plan, referred to subsequently as a batch plan, that will minimize the overall expected production costs (Eq.(1.2)). To more accurately capture the behavior of an actual re-melting operation, this simple objective is subject to a number of specific constraints. Firstly, raw materials cannot be prescribed in the batch plan in excess of the quantity available (Eq.(1.3)). Secondly, the batch plan must lead to production quantities that meet or exceed the established production target for each alloy (Eq.(1.4)). Finally, the likelihood that a batch plan leads to production that is within compositional specifications must exceed a specified probability (Eqs. (1.5) and (1.6)). This is accomplished by relating the likelihood of achieving a certain finished alloy composition to the underlying uncertainty in the chemical compositions of the raw materials, the statistical characteristics of those compositions (i.e., ε_{ik}, σ_i, and ρ_{il}), and the desired confidence limits, as established by the parameters α and β. With the understanding that the compositional constraints will not always be satisfied due to inherent uncertainty, they can be rewritten as probabilistic expressions and transformed into their deterministic equivalents.

Min:
$$\sum_i C_i X_i \tag{1.2}$$

Subject to:
$$\forall_i \ X_i \le A_i \tag{1.3}$$

$$\forall_j \ \sum_i X_{ij} = B_j \ge M_j \tag{1.4}$$

$$\forall_{j,k} \ \sum_i X_{ij}\overline{\varepsilon}_{ik} + X(\alpha)\Big(\sum_i \sum_l \rho_{\varepsilon il}\sigma_{\varepsilon i}\sigma_{\varepsilon l}\overline{\varepsilon}_i^k \overline{\varepsilon}_l^k\Big)^{1/2} \le B_j \varepsilon_{jk}^{\max} \tag{1.5}$$

$$\forall_{j,k} \ \sum_i X_{ij}\overline{\varepsilon}_{ik} + X(1-\beta)\Big(\sum_i \sum_l \rho_{\varepsilon il}\sigma_{\varepsilon i}\sigma_{\varepsilon l}\overline{\varepsilon}_{ik} \overline{\varepsilon}_{lk}\Big)^{1/2} \ge B_j \varepsilon_{jk}^{\min} \tag{1.6}$$

All other variables are defined below:

C_i = unit cost ($/T) of raw material *i*

X_i = mass (kt) purchased raw material *i (both primary and scrap)*

B_j = mass of finished good *j* produced M_j = mass of finished good *j* demanded

ε_{ik} = average mass element *k* in raw material *i*

$\varepsilon^{max}{}_{jk}$ = max. mass element *k* in finished good *j*

$\varepsilon^{min}{}_{jk}$ = min. mass element *k* in finished good *j*

A_i = mass of raw material *i* available for purchasing

X_{ij} = mass of raw material *i* used in making finished good *j*

ε_i = mean composition of raw material *i*

$\sigma_{\varepsilon i}$ = compositional standard deviation of raw material *i*

X (_) = inverse of a normalized cumulative Gaussian distribution function

α = likelihood that the actual composition will fall below the upper limit of final alloy composition

β = likelihood that the actual composition will fall above the lower limit of final alloy composition

ρ_{il} = correlation coefficient between composition of raw materials i and l (ρ_{il} = 1 when i=l)

Of these, the ones that may require further clarification are α, β, and $X()$. Individually, α and β represent the likelihood that the batch plan identified by the model will result in a composition that is lower than the upper compositional limit and greater than the lower compositional limit, respectively. X(), the inverse normalized cumulative Gaussian distribution function, characterizes the relative distance from the mean that corresponds to the designated level of likelihood.

To make this formulation more flexible to capture the metallurgical complexity of modern recycling processes it can be amended to comprehend the effects of material yield. To increase the precision of the model and to accommodate current data collection practices within industry, yield is represented by two parameters: elemental yield and gross yield. The elemental yield, Y_{ik} , represents the fractional increase or decrease of the mass of alloying element k in the melt derived from incoming material inflow i. The mechanisms that drive such mass change vary widely by element. For example, iron is expected to increase due to pick-up from processing equipment and silicon will increase due to pick-up from the furnace refractories. Other elements may decrease due to oxide formation (zinc and magnesium may form spinel), volatization, or sinking/settling of the melt. The second parameter used to capture the effects of yield is the gross melt yield, G_i, which represents total metal loss (i.e. aluminum and other elements) as a fraction of incoming raw materials i. Such loss occurs due to dross formation, spills, etc. Notably, both forms of yield are expected to exhibit some variation from batch to batch. As such, they will be incorporated into the model as stochastic parameters.

It is important to point out that while this treatment of yield does significantly increase the flexibility and the potential fidelity of the model framework, it does not capture all possible effects. In contexts where elemental interaction is larger than the natural stochastic variation of the yield, additional second order terms would need to be incorporated. Similarly, works by van Schaik and Reuter[22] [23, 24] have shown that particle size distribution and scrap conformation are key factors in metal yield and, therefore, operational decisions. The formulation presented herein does not address such effects directly. For business critical decisions where the operational decisions will affect the yield variation associated with particle size, analysts should carefully consider the explicit treatment of these issues for their specific context.

If the metallurgical yield is in fact stochastic in nature, its effect cannot be accounted for with a scalar transformation of the above formulation. Instead, the constraints on production quantity (Eq.(1.4)) and composition (Eqs.(1.5) and (1.6)) must be redeveloped. The probabilistic constraints incorporating yield can be expressed as:

$$\forall_j \ \Pr\left\{ B'_j = \sum_i X_{ij} G_i \le M_j \right\} \ge \gamma \tag{1.7}$$

$$\forall_{j,k} \ \Pr\left\{ a_{jk} = \sum_i Y_{ik} \varepsilon_{ik} X_{ij} \le B'_j \varepsilon_{jk}^{\max} \right\} \ge \alpha' \tag{1.8}$$

$$\forall_{j,k} \ \Pr\left\{ a_{jk} = \sum_i Y_{ik} \varepsilon_{ik} X_{ij} \ge B'_j \varepsilon_{jk}^{\min} \right\} \ge \beta' \tag{1.9}$$

where Y_{ik}, ε_{ik}, and G_i are random variables, $B_j^{'}$ is the actual quantity of batch j produced, a_{jk} is the actual quantity of element k in finished batch j, and γ, α' and β' are the minimum acceptable likelihood of the respective conditions being true.

The former (Eq. (1.7)) can be transformed directly into its deterministic equivalent as follows:

$$\forall_j \quad \sum_i X_{ij}\bar{G}_i + \mathrm{X}(\gamma)\sqrt{\sum_i\sum_l \rho_{Gil}\sigma_{Gi}\sigma_{Gl}\bar{G}_i\bar{G}_l} \le M_j \tag{1.10}$$

Realizing the same for the new compositional constraint requires additional manipulation. First, it is helpful to replace the product of the two random variables $Y_{ik}\varepsilon_{ik}$ with Ψ_{ik} which is also a random variable. Formally, the distribution of Ψ_{ik} is a modified Bessel function of the second kind [7]. However, for typical characteristics of elemental yield and elemental content, Ψ_{ik} can be well approximated with a normal distribution such that:

$$\Psi_{ik} \cong Y_{ik}\varepsilon_{ik} \text{ and } \Psi_{ik} \sim N(\bar{\Psi}_{ik}, \sigma^2_{\Psi_{ik}}) \tag{1.11}$$

$$\text{where } \bar{\Psi}_{ik} = \bar{Y}_{ik}\bar{\varepsilon}_{ik} \text{ and } \sigma^2_{\Psi_{ik}} = \bar{\varepsilon}^2_{ik}\sigma^2_{Y_i} + \bar{Y}^2_{ik}\sigma^2_{\varepsilon_{ik}} + \sigma^2_{Y_i}\sigma^2_{\varepsilon_{ik}} \quad [23, 24] \tag{1.12}$$

Incorporating these relationships into and rearranging Eq (1.8) yields the following probabilistic constraint:

$$\forall_{j,k} \quad \Pr\left\{\sum_i \left(\Psi_{ik} - G_i\varepsilon^{\max}_{jk}\right)X_{ij} \le 0\right\} \ge \alpha^{'} \tag{1.13}$$

Again, to simplify, it is helpful to define a new variable, $\phi^{\max}_{\mathrm{ijk}}$, such that:

$$\forall_{i,j,k} \quad \phi^{\max}_{\mathrm{ijk}} \equiv \Psi_{ik} - G_i\varepsilon^{\max}_{jk} \tag{1.14}$$

$$\text{where } \bar{\phi}^{\max}_{\mathrm{ijk}} = \bar{\Psi}_{ik} - \bar{G}_i\varepsilon^{\max}_{jk} \text{ and } \sigma_{\phi_{ijk}} = \sqrt{\sigma^2_{\Psi_{ijk}} + (\varepsilon^{\max}_{jk})^2\sigma^2_{G_i}} \tag{1.15}$$

Using these definitions it is possible to convert the probabilistic constraint Eq.(1.13) into its deterministic equivalent of the form:

$$\forall_{j,k} \quad \sum_i \bar{\phi}^{\max}_{\mathrm{ijk}}X_{ij} + X(\alpha^{'})\sqrt{\sum_i\sum_l \rho_{\phi il}\sigma_{\phi_{ijk}}\sigma_{\phi_{ljk}}\bar{\phi}^{\max}_{\mathrm{ijk}}\bar{\phi}^{\max}_{\mathrm{ljk}}} \le 0 \tag{1.16}$$

Using an identical approach it is possible to develop Eq.(1.9) into an analogous constraint on minimum compositional specifications of the form:

$$\forall_{j,k} \quad \sum_i \bar{\phi}^{\min}_{\mathrm{ijk}}X_{ij} + X(1-\beta^{'})\sqrt{\sum_i\sum_l \rho_{\phi il}\sigma_{\phi_{ijk}}\sigma_{\phi_{ljk}}\bar{\phi}^{\min}_{\mathrm{ijk}}\bar{\phi}^{\min}_{\mathrm{ljk}}} \ge 0 \tag{1.17}$$

$$\text{where } \phi^{\min}_{\mathrm{ijk}} \equiv \Psi_{ik} - G_i\varepsilon^{\min}_{jk} \tag{1.18}$$

Replacing equations (1.4), (1.5), and (1.6) with their analogs (1.10), (1.16), and (1.17), respectively, creates a schematic model that explicitly addresses uncertainty in both raw materials composition and yield.

To check the performance of the batch planning results generated by the model, Monte Carlo simulations were executed that tested the compositional acceptability of the proposed batch plan against scraps of varying composition. These simulations were carried out using Crystal Ball, an Excel based program. The Monte Carlo method uses pseudo-random numbers to statistically simulate random variables. For this case, a normal distribution around the compositional mean of each of the scraps elemental considerations (Si, Mg, Fe, Mn, Cu, Zn) was assumed and the optimal solution was tested 10,000 times. The number of batches that had any errors (i.e. final composition of finished alloys fell out of specification) was reported as the batch error rate.

3.0 Applying the Modeling Framework

The chance-constrained model presented above was utilized in two hypothetical case studies in order to: 1) test its capability in evaluating the expected recyclability of specific proposed "recycling friendly" alloys from literature[4] and 2) develop a framework that utilizes model results to *a priori* guide the design of alloys to facilitate increased recycling.

3.1 Common Data and Assumptions

For both studies, scrap types were selected to be representative of end use shipments of aluminum products in the United States and Canada. The largest categories of applications for aluminum are 1) transportation (which includes both automotive and aerospace), 2) containers and packaging, and 3) construction and building materials (Figure 3). These three categories were used to define the scrap sets used in both of the case studies and detailed in Table I; with specific scraps being selected from publicly available compositional data. The transportation scrap set is biased toward automotive related streams due to minimal current aerospace recycling and includes mixed automotive castings, high copper car radiators, segregated alloy 6061 extrusions, and automotive shredder residue (ASR), termed Zorba on the scrap market and often having large amounts of impurities. The container and packaging set includes used beverage cans (UBC), thick foil scrap (Foil), thin foil scrap (Alumifoil), and a segregated mix of alloy 1100 and 3003. Building and construction scraps include mixed aluminum wires and cables, segregated alloy 5052 clippings, clean end-of-life building siding, and segregated alloy 6063 architectural extrusions.

Finally, in addition to the three industry-specific scrap sets, a General Set of scrap was defined to be representative of the overall flow of scrap in North America. Of the old scrap consumed in 2005, UBC, castings, shredded automotives, mixed wrought scraps, and extrusions made up the majority (v. Figure 3). The General scrap set, therefore, was based on a selection of scraps from the three industry specific scrap sets that closely matched this portfolio. These include: UBC, mixed automotive castings, radiators, wire & cable scrap, and mixed turnings.

Compositional data for all scraps were estimated from EU standards[25-27] which are listed in the Appendix. The EU standards list maximum compositional specifications under which certain scrap types must fall; mean scrap compositions were estimated to be approximately 75% of these values and are listed in Table I along with their corresponding EU standard number. The elemental and gross yields are given in Table II and Table III; these were estimated from EU standards as well as input from industry experts. Elements such as silicon and iron have yields higher than one as they will generally increase due to melt contact with processing equipment and refractory. Other elements, including aluminum, will have melt loss due to dross/oxide formation, spills, etc. Notably, only very limited data is collected currently on the specifics of yield loss. Although, the figures used herein represent the collective input of three independent industry sources, detailed inquiry should be undertaken to more accurately quantify these values. Nevertheless, incorporating these values in the case analyses makes it possible to characterize the magnitude of effects attributable to yield related change.

Prices used in both case studies for primary aluminum and alloying elements were taken from USGS 2005 averages[28, 29] as shown in the Appendix. Scrap prices were estimated from various on-line scrap dealers[30] by averaging costs of similarly named and described scrap categories. Prices vary greatly by day and location, therefore cost results should be used for relative comparison only. All raw materials were assumed to be unlimited in availability in order to avoid the potential effects of limited raw materials supplies. The model framework presented herein can be used for cases of constrained scrap supply with no modification.

Within the chance-constrained formulation, the scrap raw materials were modeled with a coefficient of variation (standard deviation divided by the mean) of 50% on composition for all elements for the base case. Literature on the variability of aluminum secondary materials[7] cites coefficients of variation on elemental means ranging from 55% to as high as 3100%. Sensitivities around this number were also explored. Compositions were assumed to be perfectly uncorrelated. Collectively this set of data will be referred to as the Baseline in subsequent discussions.

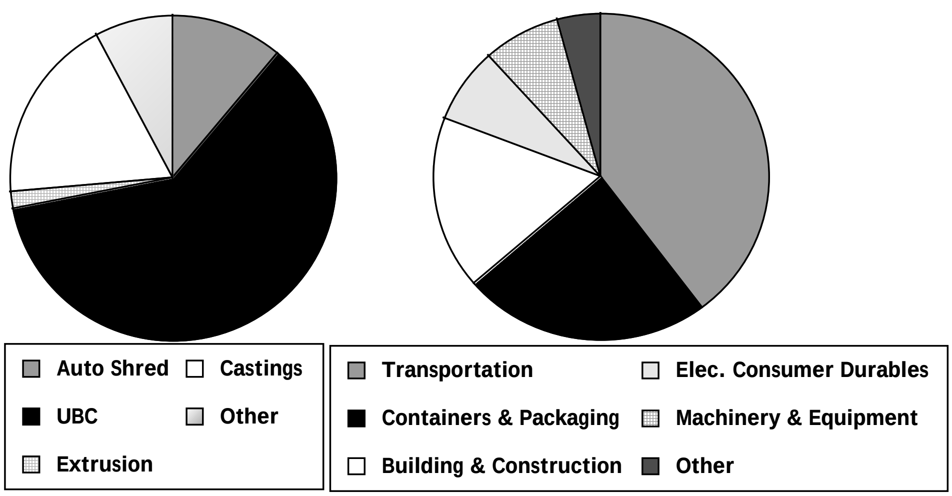


Figure 3. Percentages of old scrap consumed (total 1,154,000 metric tones) and distribution of end use shipments (total 9,699,000 metric tones) by category in the United States and Canada in 2005[31]

Table I. Average compositions for scrap sets and prices

Scrap Descriptions		Price	Si	Mg	Fe	Cu	Mn	Zn	EN #
General	Mixed Turnings	$0.74	0.0675	0.0023	0.0075	0.0263	0.0038	0.0113	13
Construction	Wire & Cable	$1.15	0.0019	0.0045	0.0030	0.0004	0.0004	0.0005	3-1
	5052 Clippings	$1.04	0.0023	0.0188	0.0038	0.0008	0.0045	0.0019	5-5
	Clean Siding	$1.02	0.0045	0.0098	0.0045	0.0015	0.0098	0.0015	5-3
	6063 Arch Ext	$1.00	0.0045	0.0038	0.0038	0.0015	0.0011	0	5-6
Automotive	Auto Castings	$0.77	0.1013	0.0023	0.0083	0.0263	0.0038	0.0090	7
	Cu-Al Radiator	$1.60	0	0	0.0053	0.3000	0	0	11
	Zorba	$0.82	0.0675	0.0038	0.0083	0.0263	0.0038	0.0090	8
	6061 Alum Ext	$0.98	0.0045	0.0038	0.0038	0.0015	0.0011	0.0019	5-6
Packaging	UBC	$0.88	0.0023	0.0098	0.0038	0.0015	0.0083	0.0004	10

	Foil	$0.95	0.0075	0.0045	0.0060	0.0060	0.0038	0.0038	6-2
	Alumifoil	$0.75	0.0075	0.0015	0.0075	0.0188	0.0030	0.0060	15
	Seg 1100/3003	$1.02	0.0071	0.0008	0.0015	0.0004	0.0004	0	4

Table II. Gross melt yield for scraps and primary

Raw Material Descriptions		Yield	Std.Dev.
General Scrap	Mixed Turnings	0.900	±0.00900
Construction Scraps	Wire & Cable	0.975	±0.00975
	5052 Clippings	0.975	±0.00975
	Clean Siding	0.975	±0.00975
	6063 Arch Ext	0.975	±0.00975
Automotive Scraps	Auto Castings	0.940	±0.00940
	Cu-Al Radiator	0.975	±0.00975
	Zorba	0.940	±0.00940
	6061 Alum Ext	0.975	±0.00975
Packaging Scraps	UBC	0.975	±0.00975
	Foil	0.975	±0.00975
	Alumifoil	0.900	±0.00900
	Seg 1100/3003	0.975	±0.00975
Primary & Alloying Elements	P1020	0.990	±0.00495
	Silicon	1	±0.00500
	Manganese	0.990	±0.00495
	Iron	1	±0.00500
	Copper	0.990	±0.00495
	Zinc	0.990	±0.00495
	Magnesium	0.990	±0.00495

Table III. Elemental yield

	Yield	Std. Dev.
Silicon	1.01	±0.0101
Magnesium	0.98	±0.0098
Iron	1.01	±0.0101
Copper	0.99	±0.0099
Manganese	0.99	±0.0099
Zinc	0.985	±0.0098

3.2 Case One Specific Data and Assumptions

The first case study involved the evaluation of three different alloy sets (R, M1, and M2), each comprising six predominant end-market aluminum alloys; one selected from each major alloy series. Set R are "recycling friendly" alloys suggested by Das[7] while Set M1 and Set M2 are the currently available alloys that most closely match the compositions of Set R. Each set was evaluated for potential scrap use within the model under conditions that would reflect production of 100 kilotonnes of each alloy for a total production of 600 kilotonnes. Because the evaluation was carried out under conditions with no limitation on the availability of raw materials, the subsequent results are independent of production scale. The scale of 100 kilotons was selected simply for statistical convenience. Maximum and minimum compositional constraints for Sets M1 & M2 are based on international industry specifications and do not reflect production targets of any specific firm; they are based on guidelines set by the Aluminum Association. These compositions are listed in Table IV.

3.3 Case Two Specific Data and Assumptions

For the second case study, two alloys, 6063 and 3004, were evaluated to identify *a priori* specification modifications that would improve potential recyclability. Compositional shadow prices were used to target which specifications should be modified (i.e., loosened or tightened); the subsequent impact on potential total scrap consumption was evaluated *post facto* in the model.

Table IV. Maximum and minimum compositional specifications for finished alloys in weight fraction[6]

	Si		Mg		Fe		Cu		Mn		Zn	
Set R	Max	Min	Max	Min	Max	Min	Max	Min	Max	Min	Max	Min
A(2XXX)	0.007	0	0.006	0	0.07	0.055	0.004	0.002	0.007	0	0.005	0
B(3XXX)	0.007	0	0.006	0	0.004	0	0.015	0.01	0.015	0.008	0.005	0
C(4XXX)	0.14	0.1	0.01	0	0.015	0.005	0.003	0	0.015	0.008	0.005	0
D(5XXX)	0.007	0	0.006	0	0.003	0	0.0035	0.0005	0.03	0.02	0.005	0
E(6XXX)	0.01	0.003	0.006	0	0.003	0	0.003	0	0.01	0.004	0.005	0
F(7XXX)	0.005	0	0.006	0	0.012	0.005	0.003	0	0.028	0.02	0.06	0.04
Set M1												
2014	0.012	0.005	0.008	0.002	0.007	0	0.05	0.039	0.012	0.004	0.0025	0
3005	0.006	0	0.006	0.002	0.007	0	0.003	0	0.015	0.01	0.0025	0
4045	0.11	0.09	0.0005	0	0.008	0	0.003	0	0.0005	0	0.001	0
5454	0.002	0	0.03	0.024	0.002	0	0.001	0	0.01	0.005	0.0025	0
6063	0.006	0.002	0.009	0.0045	0.0035	0	0.001	0	0.001	0	0.001	0
7005	0.0035	0	0.018	0.01	0.004	0	0.001	0	0.007	0.002	0.05	0.04
Set M2												
2219	0.002	0	0.0002	0	0.003	0	0.068	0.058	0.004	0.002	0.001	0
3004	0.003	0	0.013	0.008	0.007	0	0.0025	0	0.015	0.01	0.0025	0
4032	0.135	0.11	0.013	0.008	0.01	0	0.013	0.005	0.005	0	0.0025	0
5052	0.0025	0	0.028	0.022	0.004	0	0.001	0	0.001	0	0.001	0
6061	0.008	0.004	0.012	0.008	0.007	0	0.004	0.0015	0.0015	0	0.0025	0
7075	0.004	0	0.029	0.021	0.005	0	0.02	0.012	0.003	0	0.061	0.051

4.0 Results and Discussion

4.1 Case One – Evaluating Recyclability:

Comparison of "Recycling Friendly" Alloys to Representative Market Alloys

The first case study involved the evaluation of the potential for scrap use (i.e., recyclability) for three different alloy sets (R, M1, and M2), each comprised of six predominant end-market aluminum alloys; one selected from each major alloy series. Set R are "recycling friendly" alloys suggested by Das[32] while Set M1 and Set M2 are the currently available alloys that most closely match the compositions of Set R.

Table V compares the results for the Baseline conditions described above for each of three alloys sets. Results show a total improvement in potential scrap consumption of 67.9% and 65.6% respectively, with an associated decrease in primary purchased, for the scrap friendly alloy set (R) over the currently used market alloy Sets M1 & M2. These base cases were evaluated using Monte Carlo simulations to have comparably low expected error rates of 0.18%, 0.21%, and 0.25% respectively. The scrap friendly alloy set shows an associated decrease in modeled production cost of 13.4% and 13.6% over the other alloy sets.

Figure 4 shows that the batch plans for the recycling friendly alloys outperform their market counterparts for most of the alloy series investigated in terms of potential scrap use. Most notably, Alloy C(4XXX) outperforms 4032 by 10X (917%) and 4045 by almost 9X (775%); Alloy B(3XXX) outperforms 3005 by 47% and 3004 by 26%. However, the recycling friendly alloys do not consistently have higher potential scrap usage; Alloy D(5XXX) has about the same potential scrap consumption as alloy 5052 while alloy F(7XXX) is outperformed by both its comparative market counterparts, 7005 and 7075, respectively. Later sections will explore in detail the source of this underperformance.

Table V. Baseline results showing comparison of scrap friendly alloys (Set R) with current alloys (Sets M1&M2) (CC Method, 50% COV, Total Production = 600 kt)

	Alloy Set R	Alloy Set M1	% Δ R-M1	Alloy Set M2	% Δ R-M2
Scrap Use (kt)	272.5	162.3	+67.9%	164.5	+65.6%
Production Cost (M$/kt)	$1.783	$2.060	-13.4%	$2.064	-13.6%
Error Rate	0.18%	0.21%		0.25%	

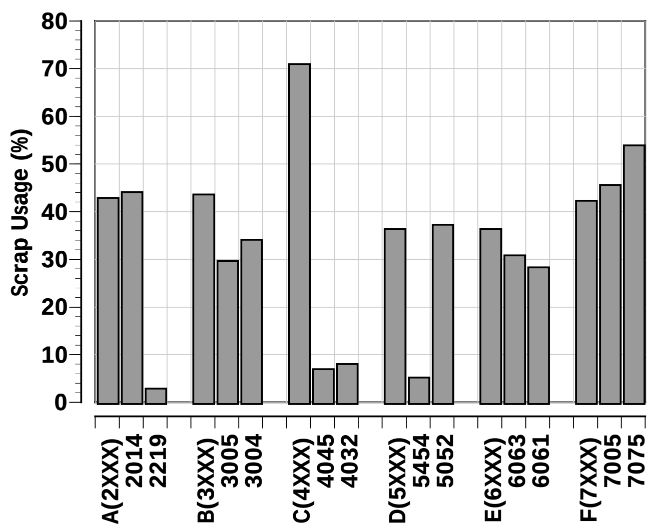


Figure 4. General scrap set consumption comparison for individual alloy sets, organized by series (CC Method, COV=50%, α=99.99%).

4.1.1 Evaluating Recyclability: Sensitivity Analysis

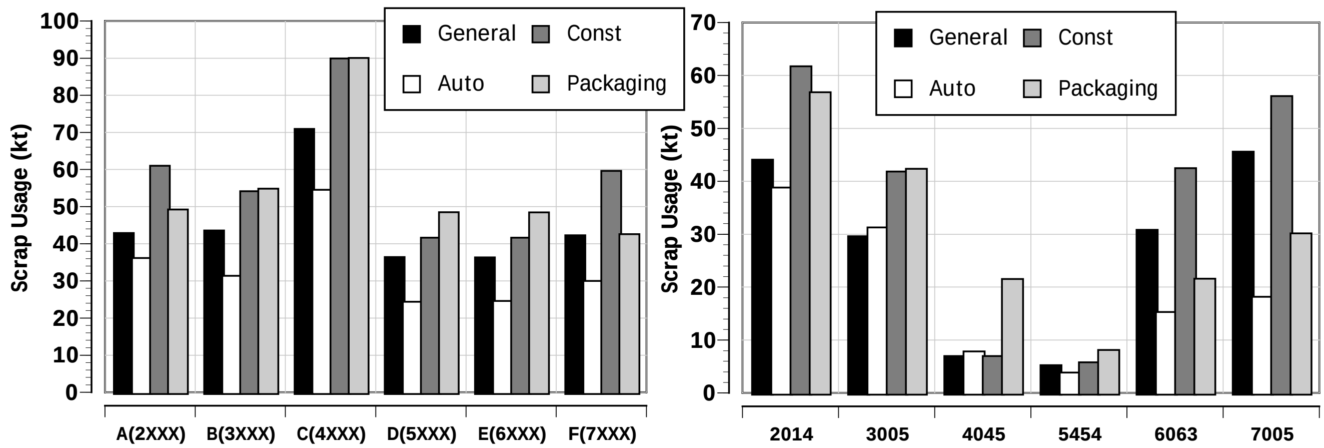
A key question with regard to any form of modeling, and particularly with optimization, is the impact of changes in model assumptions. For the problem at hand, there are many assumptions about operating conditions and raw material characteristics. The following sections will examine the impact of varying scrap sets with regard to the robustness of the ability of the recycling friendly alloys (i.e., Set R) to accommodate more scrap in their raw material portfolio than current market alloys.

Recyclability of an alloy is not only dependent on the compositional variability of the available scraps, but also the make-up of the scrap portfolio itself. Many producers, depending on the size and location of their facility, have access to scrap portfolios that will be heavy in scraps from one industry over another. To systematically explore these implications, the three candidate alloy sets were tested against three scrap portfolios, created based on the three major aluminum markets shown in Figure 3: 1) transportation, 2) containers and packaging, and 3) building and construction. The scrap portfolios, their average compositions, and modeled prices are listed in Table I. In this section, the original scrap portfolio will be referred to as General, reflecting its composition from all of the other scrap classes.

As Table VI shows, for each alloy set, the amount of scrap used is highly dependent on the available scrap "portfolio". For example, many automotive scraps go through a shredding process and therefore have a much higher accumulation of iron than other scraps[13]; one would expect the usage of these scraps to be lower than other types which is confirmed by the results. Both packaging and construction scraps have extremely low accumulation of undesirable elements and can therefore be highly utilized by all the alloy sets. Looking at the scrap consumption broken down by specific alloy (Figure 5A), one can see an even greater range of usage differences. Alloy 7005 and alloy 2014 accommodate large amounts of the construction heavy scrap in their production portfolios due to being compositionally close to clean unpainted siding. Packaging scraps, most notably used aluminum foil, have extremely low magnesium and manganese content and therefore can be utilized by alloy 4045 while that alloy can normally accommodate little to no secondary materials of other scrap types (Figure 5B).

Table VI. Total scrap material usage for the varying scrap portfolios by alloy set.

Scrap Sets	Alloy Sets		
	Alloy Set R	Alloy Set M1	Alloy Set M2
Construction	348.04	214.90	201.83
Packaging	333.61	180.55	115.54
General	272.52	162.33	164.52
Automotive	200.91	115.31	87.73



A) B)

Figure 5. Recycling friendly alloy set R (A) and market alloy (B) set M1 scrap use comparison for each different scrap "scenario"

Interestingly, not only does available scrap portfolio impact the quantity of scrap use, but it does so differentially even for analogous alloys (in the same series). As a result, the available scrap portfolio can change the relative performance of any given alloy compared to its analogs in terms of potential recyclability.

As an example, for both the Construction and General scrap portfolios, market alloy 7075 has the potential to use the most scrap of the 7-series alloys considered, while for the Automotive and Packaging scenarios, the "recycling friendly" alloy F(7XXX) can use the most scrap (Figure 6.). Recycling friendly alloy 7XXX is more compositionally restrictive for Mg compared to market alloys 7005 and 7075, while market alloy 7075 is compositionally more restrictive for Fe and Mn compared to the recycling friendly alloy (see Table IV). For the Automotive-heavy scrap portfolio case, one can see from

Table VII that the recycling friendly alloy is able to utilize more Zorba and 6061 aluminum extrusion than market alloy 7075; these scraps have fairly high iron and magnesium content. For the Construction-heavy scrap portfolio case, one can see that market alloy 7075 utilizes more wire and cable scrap compared to the other two alloys. Wire and cable scrap are desirable due to their low silicon content (cf. Table I), however, due to their high usage the magnesium becomes the constraining element. This allows alloy 7075 to accommodate more secondary materials in its portfolio overall.

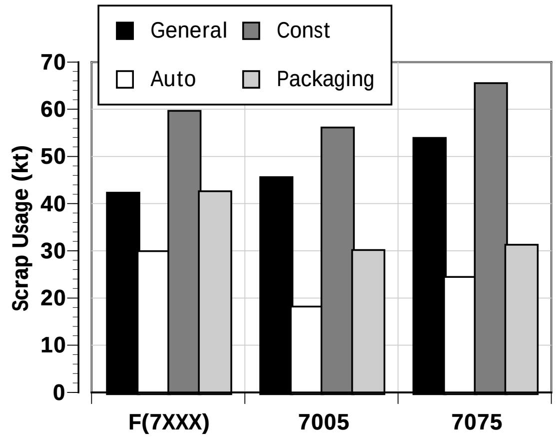


Figure 6. Comparison of scrap used in the production portfolio of the 7XXX series alloys for each of the scrap scenarios

Table VII. Scrap usage (in kilotons) for 7XXX series alloys

Automotive Set	7XXX	7005	7075	Construction Set	7XXX	7005	7075
Auto Castings	0.1	0.1	0.1	Wire & Cable	25.2	26.8	37.8
Cu-Al Radiator	0.2	0	0.7	5052 Clippings	1.7	8.5	4.7
Zorba	0.1	0.1	0.1	Clean Siding	5.8	7.3	7.7
6061 Alum Ext	29.4	18.0	23.5	6063 Arch Ext	26.6	13.5	15.3

Similar results can be shown for the 5XXX alloys. D(5XXX) outperforms its market counterparts for the Automotive- and Packaging-heavy scrap portfolios, while for the General- and Construction-heavy portfolios, alloy 5052 can accommodate the most secondary materials in its production portfolio (Figure 7). In this case, for the Packaging-heavy portfolio, Seg 1100/3003 is desirable because it has a low iron content compared to the other scraps (cf. Table I), however, silicon becomes a constraining element in the production portfolio and therefore the recycling friendly alloy can consume more due to its less restrictive silicon specification. On the other hand, for the General portfolio, alloy 5052 has the potential to use more Wire and Cable scrap (Table VIII) in its production portfolio because it is less compositionally restrictive in magnesium and manganese when compared to D(5XXX).

Ultimately, it is clear that the recycling performance of a specific alloy can be strongly dependent on the operational context in which it is applied. Mathematical programming, like the chance-constrained model used herein, provides rapid, quantitative insight without the need for expensive and time-consuming experimentation. Nevertheless, given the range of potential operational settings (i.e. available scrap types, compositional variability, raw material prices, etc.) and the continuum of possible compositional modifications, *post facto* evaluation, even through a model, may not make effective alloy design tractable. Instead, the alloy designer needs insight into what modifications can provide the most benefit. The next section, through the use of a case study, explores the use and value of that information, referred to as a shadow price, to direct the development of more recyclable alloys.

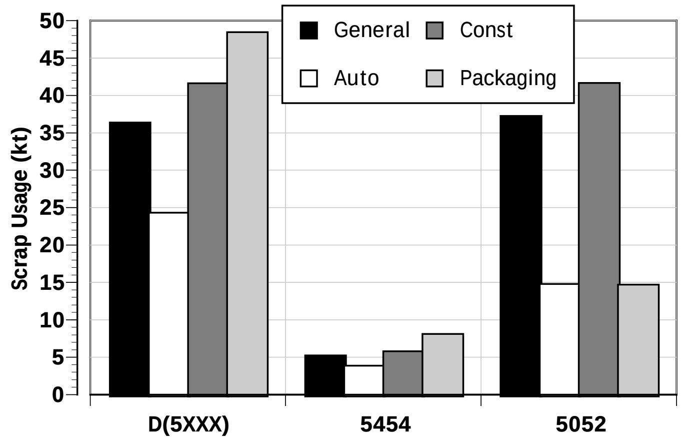


Figure 7. Comparison of scrap used in the production portfolio of the 5XXX series alloys for each of the scrap scenarios

Table VIII. Scrap usage (in kilotons) for 5XXX series alloys

Packaging Set	5XXX	5454	5052	General Set	5XXX	5454	5052
UBC	16.6	2.3	2.9	UBC	14.5	2.3	2.9
Foil	4.4	0.2	3.1	Auto castings	1.2	0	0.0
Alumifoil	2.3	0	1.0	Cu-Al Radiator	0.2	0	0.1
Seg 1100/3003	25.0	5.7	7.7	Wire and Cable	18.6	2.9	34.0
Mixed turnings	0.1	0	0	Mixed turnings	1.9	0	0.3

4.2 Case Two – Designing for Recyclability: Using Compositional Shadow Prices

As has been shown previously[33], the mismatch between scrap composition and alloy compositional specifications creates the primary technological constraint on scrap use. A clear strategy to facilitate recycling is to modify alloy specifications such that production can accommodate more scrap. Unfortunately, the trivial solution of broadening all compositional specifications is sure to alter alloy materials properties. Instead, the alloy designer must selectively alter specifications, relaxing some, while tightening others, all within performance specifications. Case Two explores the use of model outputs to guide the *a priori* modification of alloy specifications to improve potential for scrap use. Simple examples from Case One can serve to illustrate the challenge of realizing an effective design in the absence of such guidance.

Consider the relative performance of the 4XXX and 5XXX alloys as described in the previous section (i.e., Alloy C had the highest potential for scrap use of the 4XXX alloys while 5052 had the highest potential for scrap use of the 5XXX alloys (v. Figure 4**)** and their specifications as shown in Figure 8. Examining Figure 8, Alloy C, compared to its market equivalent 4XXX alloys, has a broader specification range for all elements with the exception of Cu and a higher maximum specification range for all elements except for Cu and Mg. This is in stark contrast to alloy 5052 which, compared to the other 5XXX alloys considered, has the highest potential for scrap use but neither the broadest nor highest maximum specification with the exception of Fe. These observations lead to the following critical questions: Is range broadening a key element of improving recyclability? Which specifications can be lowered? Which can be raised? Is there a way to rationalize the alloy design process?

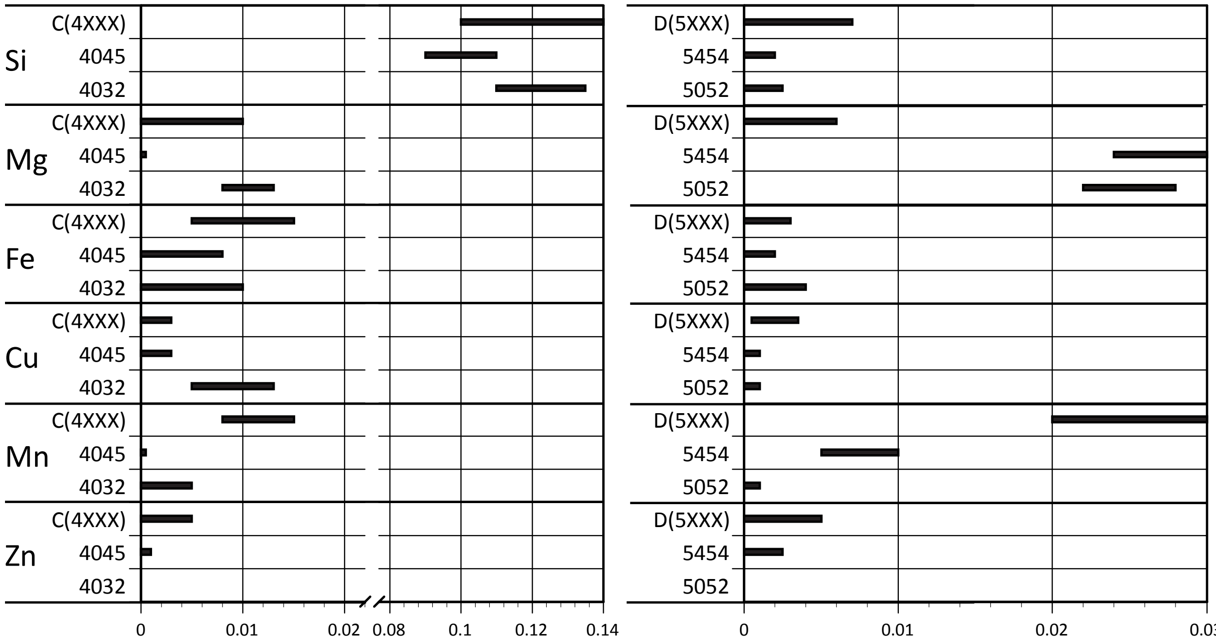


Figure 8. Schematic representation of alloy compositional specification windows for the 4XXX and 5 XXX series alloys of all three sets

As shown earlier in this paper, mathematical programming models would allow alloy designers to project the recyclability impact of a specific modification. With current specifications comprehending nearly two dozen elements, it is not practical to iterate through every possible specification. Fortunately, the type of model presented in this paper also generates a set of information that can direct the design process. As described above (see section 2.1), shadow prices identify those specifications with both the most and least impact on recyclability. Specifically, the magnitude and sign of the shadow prices on composition indicates how the production cost would change if the compositional specifications were tightened or loosened. Armed with that information, the design process should become more efficient.

It is no surprise that, for a model either minimizing raw material cost or maximizing scrap use, more of the binding compositional constraints are maximums (e.g., 30 of 52 for the recycling friendly alloy set); the amount of contaminants in a scrap usually determines how much dilution with primary aluminum is required and is therefore the major limiting factor. The shadow prices on magnesium, copper, and manganese are typically higher because these three alloying elements are the most expensive (>$2,000/tonne within the cases studied herein) and therefore have the highest impact on the production cost.

Although forensic use of shadow prices is informative, a prospective framework can be implemented to systematically and efficiently target for development alloy specifications that provide the most significant improvements in potential for increased scrap reuse and reduced production cost.

For alloy 6063, the largest compositional constraint is that on the maximum specification for magnesium (Table IX). One would therefore propose a “recycling friendly” alloy with a relaxed constraint on magnesium. This alloy is the same as market alloy 6063 but the compositional constraints are modified slightly by changing the maximum magnesium specification, this modification ranges from 10% to 100% of the original Aluminum Association (AA) specification of 0.90 wt.%. Specifically, a starting value of 10% of the original Aluminum Association (AA) magnesium maximum specification corresponds to a new maximum of 0.49 wt.%. Expanding this specification from 10% to 100% of the AA specification results in a 16-fold increase in scrap utilization. Increasing the specification beyond the original AA specification could result in even higher scrap utilization; however, these changes may be less feasible due to processing and property restrictions. Figure 9A illustrates how loosening this constraint, while still remaining within the AA specification, can enable increased scrap utilization in the case study alloy's production portfolio.

It is intuitive that relaxing compositional constraints make it possible for an alloy to accommodate more scrap in its optimal production portfolio; however, it is also possible to tighten certain constraints without compromising scrap use. Compositional shadow prices indicate which of the constraints could be tightened. Looking at the compositional shadow prices in Table IX, one would expect that the specifications on silicon and zinc for 6063 could be tightened without negative impact on scrap usage. A compositional shadow price of zero indicates a non-binding constraint; the lowest shadow prices therefore correspond to the least binding compositional constraints. Figure 9B shows that this hypothesis is correct for specification tightening of 0 to 60% for both Si and Zn. The high shadow prices on copper and manganese would indicate that tightening this constraint may have a large effect on scrap usage. However, iron actually has the largest impact on scrap utilization when tightening its specification, most likely due to pick-up during processing and melting (this is captured by a value larger than 1 for yield, cf. Table III). Tightening the Fe constraint up to 40% still has no negative effect on scrap consumption, however, tightening past this point (up to 95%) results in a rapid decrease in scrap utilization. Si, Cu, Mn, and Zn all have non-zero compositional shadow price so some effect on scrap use would be expected. One can see that tightening these constraints beyond 60% begins to have a significant impact on the scrap utilization.

Table IX. Compositional shadow prices for maximum specifications for 6XXX and 3XXX series market alloys

	Example 1		Example 2	
Element	Alloy 6063	Alloy 6061	Alloy 3005	Alloy 3004
Si	0.9	7.4	7.7	9.7
Mg	74.3	81.4	83.8	83.1
Fe	2.0	2.0	2.0	2.0
Cu	20.5	0.7	0.8	0.6
Mn	29.9	8.4	0.0	0.0
Zn	1.2	1.2	1.2	1.2

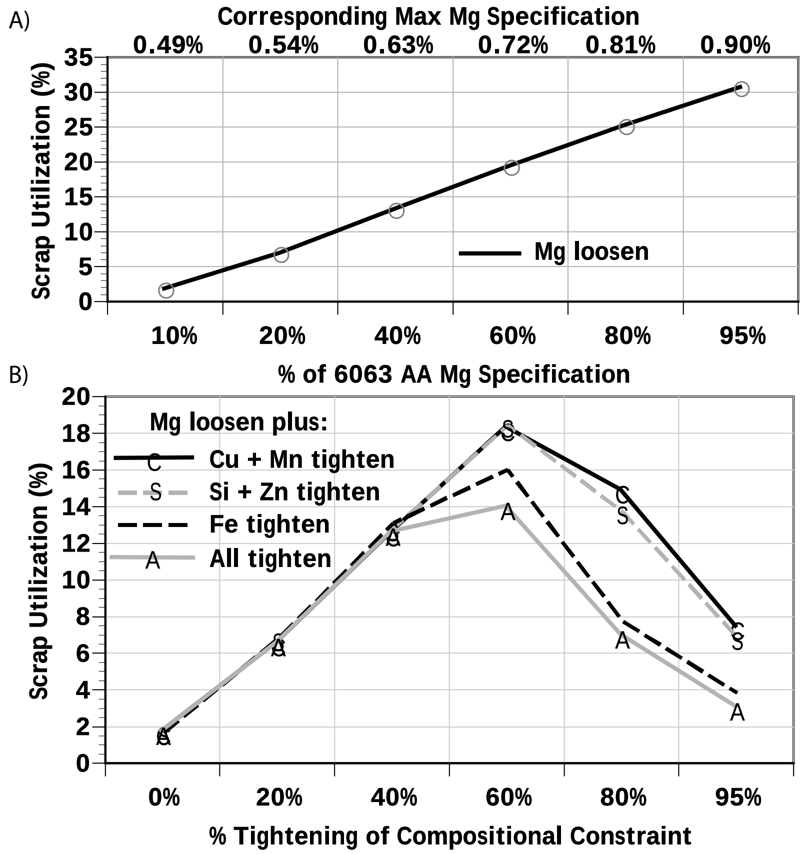
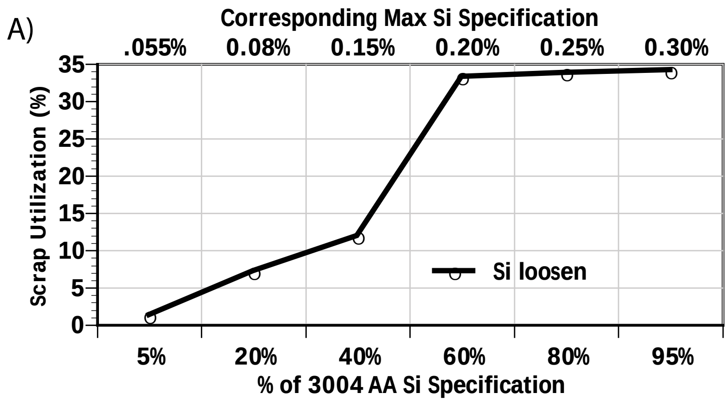


Figure 9. A) Improvement in scrap consumption of loosening Mg constraints on alloy 6063, B) Effect on scrap consumption of now tightening other constraints in conjunction with loosening the Mg constraint

One of the examples where the modifications to make a more "recycling friendly" alloy were not successful for every scrap type were for the 3XXX series alloys; this is a case where the market alloy could accommodate more scrap than the proposed recycling friendly alloy for one for the cases. By looking at the compositional shadow prices on the maximum specifications for the 3XXX series market alloys (cf. Table IX), one can see that magnesium and silicon have the highest shadow prices for both alloy 3005 and alloy 3004. One would therefore propose a "recycling friendly" alloy with relaxed constraints on those elements. A compositional shadow price of zero indicates a non-binding constraint.

Figure 10A shows the scrap consumption for the representative market alloy (3004) and the modified case study alloys designed using shadow price information. These alloys are the same as market alloy 3004 but the compositional constraints are modified slightly by changing the maximum silicon specification, this modification ranges from 5% to 100% of the original Aluminum Association (AA) specification. Specifically, for alloy 3004 the original maximum silicon specification was 0.3 wt% (cf. Table IV); a specification window size of 5% corresponds to a new maximum specification of 0.055 wt% while a window size of 60% corresponds to a maximum specification of 0.2 wt%. The minimum silicon specification remains the same, thereby increasing the specification window size up to the original value. Expanding the silicon specification from 5% to 40% of the original AA specification results in an 8-fold increase in scrap utilization. Further expanding from 5% to 100% (of the original AA specification) increases the scrap utilization by 25X.

Examining the shadow prices for alloy 3004 (cf. Table IX), one hypothesizes that tightening the constraints on Mn, Zn, and Cu would have less of an impact than tightening Mg and Fe which have higher maximum shadow prices. Figure 10B shows how scrap usage is impacted if the Si constraint were loosened as shown previously but in conjunction with tightening other constraints. One can see that the maximum constraints on Mn, Cu, and Zn can be tightened (up to 90%) with no negative impact on scrap usage. The constraint on Fe must be tightened past 60% in order to begin to affect scrap usage, however, even at an 80% more compositionally restrictive value, there is still a positive improvement in scrap use. Tightening the magnesium constraint has a strong effect on scrap consumption as one would expect from its higher shadow price. Tightening the Mg constraint beyond 40% results in less scrap use in the modified 2014 alloy than with no modification. The line labeled "A" shows the aggregate effect of tightening all of the compositional constraints except Si.



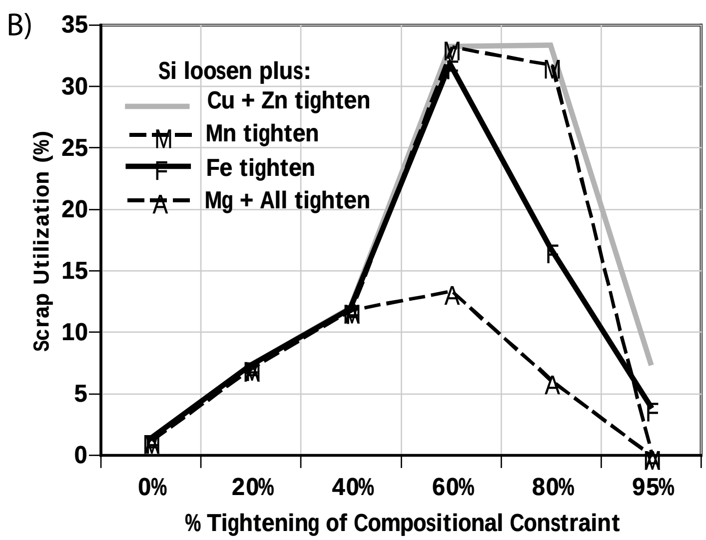


Figure 10. A) Improvement in scrap consumption of loosening Si constraints on alloy 3004, B) Effect on scrap consumption of now tightening other constraints in conjunction with loosening the Si constraint

The compositional shadow prices for magnesium and silicon for these modified alloys are shown in Figure 11; notably, the shadow prices on magnesium grow as the shadow prices on the silicon shrink. This would indicate that as the silicon specification becomes less and less constraining, the magnesium specification becomes the major factor preventing further scrap usage. After the 40% tightening, the shadow price on magnesium grows to be larger than the original shadow price on silicon, thus the negative impact on total scrap consumption.

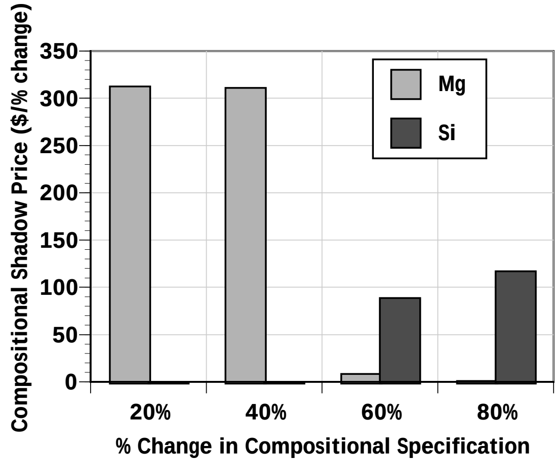


Figure 11. Change in compositional shadow prices as the constraints on magnesium are loosened and the constraints on silicon are tightened.

Shadow prices provide information on what elemental specification modifications may provide the largest impacts on scrap use (both positive and negative). The above examples are scenarios for alloy design that illustrate how modifications in compositional constraints can allow for increased scrap consumption. The large number of elemental considerations of today's aluminum alloys coupled with the often volatile state of the secondary materials market make alloy design for recycling an increasingly complex and challenging task. The model/tool presented in this paper aids the alloy designer by considering both compositional uncertainty of secondary materials and the impact their use has on alloy recyclability. The sensitivity analysis that accompanies the optimal production portfolio solutions can guide designers in terms of targeting which specification constraints could be relaxed or tightened.

5.0 Conclusions

Growing industrial awareness of resource scarcity and environmental impact has highlighted the steadily increasing consumption of metals and materials in production. A key strategy for enabling a shift to more sustainable use of materials will be increased recycling. Although reaching full recycling potential will likely require changes throughout any given materials system, one strategy that may play an important role is the redesign of alloys to accommodate more scrap. Realizing such redesign will require effective tools to evaluate an alloy's potential recycling performance; without such tools, redesign can only proceed by expensive trial-and-error. This paper has explored the use of a modeling framework, specifically a chance-constrained optimization framework, as such a systematic method to (1) evaluate an alloy's ability to accommodate recycled materials (scrap) in its production portfolio and (2) proactively identify the most effective alloy modification strategies that can drive increased potential scrap use. Additionally, this paper extended previous work in this space by presenting a schematic algorithm for explicitly incorporating uncertain metal yield into the analyses of alloy design specifically, and recycler operational decisions more broadly.

In the case presented here, the model was shown to be effective at differentiating the potential scrap usage of a set of suggested "recycling friendly" alloys particularly as production context shifted across different scraps sets. The specifications for these alloys as suggested in the literature were generally shown to enable increased scrap usage, although this improvement was not uniform across all alloy series. This improvement in secondary material utilization was shown to be context dependent on both the product the alloy is replacing as well as the scraps that are available for its production.

The chance-constrained optimization framework was also shown to be useful in guiding the initial alloy design process in regards to which compositional specifications should be targeted for modification in order to increase recyclability. With regard to this guiding design, this paper extends previous discussions [4] by exploring in detail how sensitivity analysis information actually correlates with potential scrap use performance and how both the sensitivity analysis information and the associated potential scrap use effect changes with individual and coordinated specification modifications. The case analyses suggest that real potential exists for increasing potential scrap use through alloy redesign while remaining within established compositional specifications.

Both the model and cases discussed herein are intended to be schematic in nature. Much work still remains to capture the metallurgical complexity of the recycling process; nevertheless, the results presented show that this framework holds promise to be a valuable tool in the metallurgists toolkit. This is especially important for materials engineers because evaluating all possible specification combinations is not practical for efficient decision making. In addition to being highly efficient, this method makes use of the current tools and technologies in place for aluminum batch planning and therefore requires no additional capital investment for rapid implementation. In the end, tools built around frameworks like this can aid the strategic decision-making of today's materials designers, enabling recycling performance to become an aspect of the design process. In the end, that design process is still dependent on traditional and emerging methods to identify alloys that will satisfy demanding physical performance requirements. Nevertheless, efficient design of resource-conscious materials will require analytical tools capable of projecting the impact of design choices on recycling performance.

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6.0 References

[1] T. E. Graedel, B. R. Allenby, Industrial ecology, Prentice Hall, Upper Saddle River, NJ, 2003, p. 363.

[2] R. A. Frosch, N. E. Gallopoulos, Scientific American 261 (1989) 144-152.

[3] G. A. Keoleian, K. Kar, M. M. Manion, J. W. Bulkley, Industrial Ecology of the Automobile: A Life Cycle Perspective, Society of Automotive Engineers, Inc., Warrendale, PA, 1997, p. 148.

[4] T. Kelly, D. Buckingham, C. DiFrancesco, K. Porter, T. Goonan, J. Sznopek, C. Berry, M. Crane, Historical Statistics for Mineral and Material Commodities in the United States, USGS, 2004, p.1-5.

[5] F. Hobbs, N. Stoops, Demographic Trends in the 20th Century, Census 2000 Special Reports Series CENSR-4, vol US Census Bureau, Washington, DC, 2002.

[6] A. Gesing, Journal of Materials August 2004 (2004) 18-27.

[7] S. K. Das, Emerging Trends in Aluminum Recycling: Reasons and Responses, in: T. J. Galloway, TMS (The Minerals, Metals & Materials Society, vol Light Metals 2006, San Antonio, Texas, 2006, p. 911-916.

[8] J. W. Sutherland, K. L. Gunter, D. Allen, D. Bauer, B. Bras, T. G. Gutowski, C. Murphy, T. Piwonka, P. Sheng, E. W. Thurston, International Journal of Vehicle Design 35 (2004).

[9] R. Woodward, Where next wrought aluminium alloys?, in: Aluminium Today, vol 21, 1997.

[10] J. R. Lund, G. Tchobanoglous, R. P. Anex, R. A. Lawver, Journal of Environmental Engineering 120 (1994) 1082-1094.

[11] J. A. Stuart, Q. Lu, IEEE Transactions on Electronics Packaging Manufacturing 23 (2000) 314-320.

[12] J. S. Shih, H. C. Frey, European Journal of Operational Research 83 (1995) 452-465.

[13] R. Kirchain, A. Cosquer, Resources Conservation & Recycling 51 (2007).

[14] G. Gaustad, P. Li, R. Kirchain, Resources Conservation & Recycling 52 (2007) 180-207.

[15] A. van Schaik, M. A. Reuter, U. M. J. Boin, W. L. Dalmijn, Minerals Engineering 15 (2002) 1001-1016.

[16] M. A. Reuter, A. van Schaik, O. Ignatenko, G. J. de Haan, Minerals Engineering 19 (2006) 433-449.

[17] A. van Schaik, M. A. Reuter, Resources Conservation & Recycling 40 (2004) 301-328.

[18] R. d. Neufville, Applied Systems Analysis: Engineering Planning and Technology Management, McGraw-Hill Publishing Company, New York, 1990, p. 470.

[19] A. Cosquer, R. Kirchain, TMS: The Minerals, Metals, and Materials Society AA3 (2003).

[20] A. Cosquer, Optimizing the Reuse of Light Metals from End-of-Life Vehicles, Thesis: Engineering Systems Division, Massachusetts Institute of Technology, Cambridge, MA, 2003, p. 98.

[21] A. van Schaik, M. A. Reuter, K. Heiskanen, Minerals Engineering 17 (2004) 331-347.

[22] M. D. Springer, The algebra of random variables, Wiley, New York, 1979, p. 470.

[23] L. W. Cornwell, L. A. Aroian, V. S. Taneja, Journal of statistical computation and simulation 7 (1978) 123-131.

[24] L. A. Aroian, V. S. Taneja, L. W. Cornwell, Communications in statistics, theory, and methods 7 (1978) 164-172.

[25] A. M. Market, Non-ferrous scrap prices, 2006.

[26] Recycling Xchange, www.recyclingxchange.com, 2006.

[27] Global Scrap, www.globalscrap.com, 2007.

[28] R. D. Peterson, Scrap Variability and its Effects on Producing Alloys to Specification, in: TMS: The Metals, Minerals, and Materials Society, Light Metals 1999.

[29] Z.-K. Liu, Effect of Impurities on Alloys, in: I. T. Program, Energy Efficiency and Renewable Energy, US Department of Energy, Washington, DC, 2003.

[30] P. Plunkert, Aluminum, in: US Geological Survey Minerals Yearbook, USGS, 2005, p.20.

[31] A. Gesing, Journal of Materials 53 (2001).

[32] G. Gaustad, P. Li, R. Kirchain, Managing Raw Materials Compositional Uncertainty: Chance Constrained Modeling for Alloy Production, in: Materials Science and Technology (MS&T) 2006, Cincinnati, OH, 2006.

[33] EN 13920: Aluminium and Aluminium Alloys-Scrap, in: B. B. Standards, European Committee for Standardization, 2003.

7.0 Appendix

Table X. European standard designation numbers and scrap type descriptions

EU#	Scrap Description
3-1	Wire and cable scrap-unalloyed Al
4	Scrap consisting of one single wrought alloy
5-3	Scrap consisting of 3XXX series wrought alloys
5-5	Scrap consisting of 5XXX, high Mg wrought alloys
5-6	Scrap consisting of 6XXX series wrought alloys
6-2	Scrap consisting of two wrought alloys – Grade A
7	Scrap consisting of castings
8	Scrap consisting of non-ferrous materials from shredding processes
10	Scrap consisting of used aluminum beverage cans
11	Scrap consisting of aluminum-copper radiators
13	Mixed turnings consisting of two or more alloys
14	Scrap from post-consumer aluminum packaging
15	Decoated aluminum scrap from post-consumer packaging

Table XI. Prices of primary materials and alloying elements

Primary Materials & Alloying Elements	Price ($/T)
P1020- Primary Al	$2,410
Silicon	$1,540
Manganese	$2,630
Iron	$440
Copper	$3,300
Zinc	$1,210
Magnesium	$2,700