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Identifying Scrap Friendly Alloys using Chance Constrained Modeling

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Abstract

A key element for realizing long term sustainable use of any metal will be a robust recycling industry. To expand secondary production, it is necessary to reduce the barriers to return, collect, and process recycled materials. One such barrier is the mismatch between the composition of returning post-consumer scrap and current alloy specifications. This paper examines the use of linear optimization models to provide detailed strategies for secondary metal processors, remelters, and product designers in their selection and specification of alloys. A case study involving typically recycled aluminum components is presented to evaluate a set of scrap friendly alloys proposed by the authors[1]. Specific focus will be given to the impact of scrap compositional uncertainty in the alloy design process. Initial results show that utilization of these new techniques provides a systematic approach to inform alloy designers on business-critical decisions that provide both increased scrap consumption and related economic benefit.

Introduction

Modeling tools are available and broadly applied to support the decisions of secondary batch planners. Many producers make use of linear optimization (LO) techniques[2]. These LO models can improve decisions not only about raw materials mixing, but also purchasing, upgrading, and sorting of secondary materials[3-7]. Analytical approaches may be used within such tools to embed consideration of uncertainty in the decision-making, but generally this occurs through the use of statistical analyses that are used to forecast expected outcomes. Although this combination of statistical analysis and modeling can be powerful, it suffers from two fundamental limitations. First of all, assessments based on mean expected conditions implicitly assume that deviations from those conditions have symmetric consequences. For many production related decisions within the cast-house, the consequences of errant decisions are inherently asymmetrical. This is obviously the case for compositional errors, where corrective measures rely upon either additives or dilutants with sometimes significantly different costs. Additionally, deterministic approaches generally do not provide proactive mechanisms to modify production strategies as prevailing conditions evolve.

To address these shortcomings, the authors have previously proposed modifications[8] to traditional LO models used for batch planning that allow decisions to be made using a more rich set of statistical information. Specifically, these modifications are referred to as a chance-constrained (CC) formulation. The CC formulation allows a model to be constructed that embeds not only mean-based information, as with traditional LO models, but also some measure of dispersion (i.e., sample variance). This paper will focus on the strategic use of this CC formulation to 1) characterize the performance of proposed alloy modifications to increase scrap reuse potential and 2) identify opportunities to further improve those alloy specifications.

Methods

Chance Constrained Optimization Model

Stochastic programming methods including chance constrained variants were first formulated by Charnes and Cooper[9] as mechanisms to embed a more rich set of statistical information into optimization based decision models. This method relates the desired level of confidence to the underlying standard deviations observed in the sampled raw materials. With the understanding that the compositional constraints will not be satisfied always due to inherent uncertainty, they can be rewritten as probabilistic expressions and transformed into their deterministic equivalents. For mathematical details, please refer to[8]. The chance constrained problem for both batch planning and to evaluate strategic recycling opportunities for the firm can be formulated as follows as a linear optimization model. The mathematical definition of the model is given in Equations (1) through (6). The goal of this model is to minimize the overall expected production costs (cf. Equation(1)) while meeting finished good compositional specifications through optimal and efficient use of primary and secondary raw materials. Equations (2) and (3) ensure that raw materials cannot be used in excess of quantities physically available. Equation (4) ensures that production meets or exceeds the established target level for each product.

$$\textbf{Min:} \quad \sum_s C_s P_s + \sum_p C_p P_p \quad \textbf{(1)}$$

$$\textbf{\textit{Subject to}:} \quad P_s \le A_s \quad \textbf{(2)}$$

$$P_p \le A_p \quad \textbf{(3)}$$

$$\sum_s P_{sf} + \sum_p P_{pf} = B_f \ge M_f \quad \textbf{(4)}$$

For each alloying element *c,* the composition of each alloy produced must meet production specifications:

$$\sum_s P_{sf} U_{sc} + \sum_p P_{pf} U_{pc} + X(\alpha)(\sum_s \sum_t \rho_{st}\sigma_s\sigma_t x_s x_t)^{1/2} \le B_f U_{fc}\alpha \quad \textbf{(5)}$$

$$\sum_s P_{sf} L_{sc} + \sum_p P_{pf} L_{pc} + X(1-\beta)(\sum_s \sum_t \rho_{st}\sigma_s\sigma_t x_s x_t)^{1/2} \ge B_{fz} L_{fc}\beta \quad \textbf{(6)}$$

All other variables are defined below:

C_s	= unit cost (\$/T) of scrap material *s*	C_p	= unit cost of primary material *p*
P_s	= amt. (kt) purchased scrap material *s*	P_p	= amt. (kt) purchased primary material *p*
B_f	= amount of finished good *f* produced	M_f	= amount of finished good *f* demanded
U_{sc}	= max. amt. element *c* in scrap material *s*	L_{sc}	= min. amt. element *c* in scrap material *s*
U_{pc}	= max. amt. element *c* in primary material *p*	L_{pc}	= min. amt. element *c* in primary material *p*
U_{fc}	= max. amt. element *c* in finished good *f*	L_{fc}	= min. amt. element *c* in finished good *f*
A_s	= amount of scrap material *s* available for purchasing		
A_p	= amount of primary material *p* available for purchasing		
P_{pf}	= amount of scrap material *s* used in making finished good *f*		

Monte Carlo Simulation

To test the performance of the batch mixing solutions provided 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 (i.e. not truly random in the sense that they are generated by numerical algorithms) 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 recorded.

Case Study

The chance constrained formulation was utilized to evaluate scrap friendly alloys in a hypothetical case study. Specifically, the case involved the production of three different sets of six predominant end-market aluminum alloys; one selected from each series. Set A are recycling friendly alloys suggested by Das[1] while Set B and Set C are the currently available alloys that most closely match the compositions of Set A. Production was required to meet the demand of 100 kt each alloy for a total production of 600 kt. Maximum and minimum compositional constraints for Sets B & C 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 I. Scrap types and compositions were taken from EU standards[10]; these values are listed in Table II. Prices for primary aluminum and alloying elements were taken from USGS 2005 averages[11] while scrap prices were estimated from [12] (Table III). 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 of 50% for the base case on composition for all elements. Sensitivities around this number were also explored. Because of the novelty of the chance-constrained method, results are compared against those of more traditional deterministic models. The details of this mode, referred to herein as window-narrowing can be found in [8]. Two key features of this deterministic model is 1) the amount by which the actual specification is reduced or narrowed to prevent compositional error (referred to as window-narrowing) and 2) the width of the compositional range assigned to the scrap material, stated in terms of the number of standard deviations from the mean. For the deterministic window narrowing runs, the maximum and minimum scrap compositions were set to be two standard deviations from the mean values reported in Table II unless otherwise noted. For chance constrained runs, compositions were also assumed to be perfectly uncorrelated.

Table I. Maximum and Minimum Compositional Specifications for Finished Alloys in weight fraction[13]

Set A	Si Max	Si Min	Mg Max	Mg Min	Fe Max	Fe Min	Cu Max	Cu Min	Mn Max	Mn Min	Zn Max	Zn 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 B												
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 C												
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

Table II. Average compositions for scraps in weight fraction

Scraps	Si	Mg	Fe	Cu	Mn	Zn
UBC	0.00225	0.00975	0.00375	0.0015	0.00825	0.000375
Mixed auto castings	0.10125	0.00225	0.00825	0.02625	0.00375	0.009
Cu- alum radiator	0	0	0.00525	0.3	0	0
Wire and cable scrap	0.001875	0.0045	0.003	0.000375	0.000375	0.000525
Mixed turnings	0.0675	0.00225	0.0075	0.02625	0.00375	0.01125
Litho sheets	0.006	0	0.006375	0.00125	0.006375	0.00075

Table III. Prices of primary materials and alloying elements[11] and representative scraps[12]

Primary Materials & Alloying Elements	Price ($/kt)	Scraps	Price ($/kt)
P1020- Primary Al	$2.41	UBC	$1.00
Silicon	$1.54	Mixed auto castings	$0.86
Manganese	$2.63	Cu- alum radiator	$0.29
Iron	$0.44	Wire and cable scrap	$0.32
Copper	$3.30	Mixed turnings	$0.24
Zinc	$1.21	Litho sheets	$0.29
Magnesium	$2.70		

Results and Discussion

Base Case Results

Table IV compares the results for the chance constrained (CC) method with 50% coefficient of variation (COV) for each of three alloys sets. Results show a total improvement in scrap consumption of 47.9% and 55.5% respectively, with an associated decrease in primary purchased for the scrap friendly alloy set over currently used alloy Sets B & C. These base cases have comparably low error rates of 0.20%, 0.38%, and 0.30% respectively. The scrap friendly alloy set shows an associated improvement in production cost of 14.1% and 17.3% over the other alloy sets. One can see from Figure 1 that the recycling friendly alloys outperform their market counterparts for most of the alloy series. Most notably Alloy C(4XXX) outperforms 4032 by 4X and 4045 by 10X; Alloy A(2XXX) outperforms 2219 by 6X and has slightly higher scrap consumption than 2014 (approximately 4%). However, the recycling friendly alloys do not have higher scrap usage across the board; Alloy F(7XXX) has about the same scrap consumption as alloy 7075 while both alloys B(3XXX) and D(5XXX) are outperformed by their comparative market counterparts, 3005 and 5052, respectively.

Table IV. Base case results showing comparison of suggest scrap friendly alloys (Set A) with current alloys (Sets B&C) (50% COV, Total Production = 600 kt)

	Alloy Set A	Alloy Set B	A-B Difference	Alloy Set C	A-C Difference
Scrap Use (kt)	335.93	227.09	47.9%	216.00	55.5%
Production Cost ($/kt)	$1.647	$1.916	-14.1%	$1.991	-17.3%
Error Rate	0.20%	0.38%		0.30%	

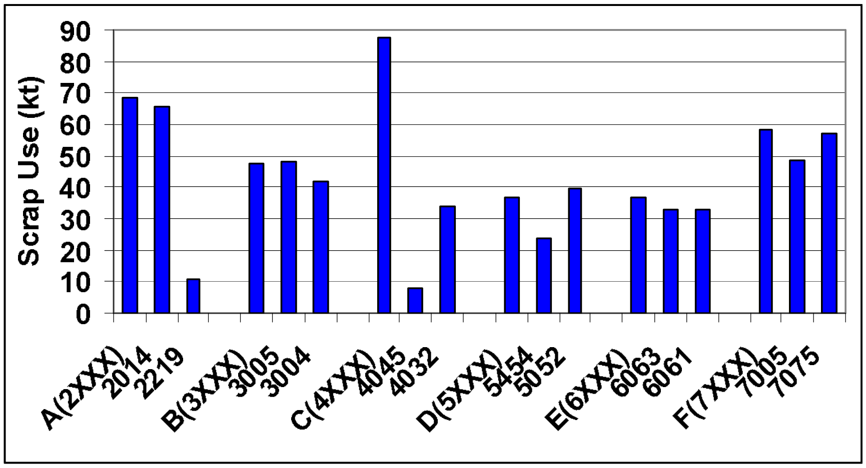

Figure 1. Scrap use shown for individual alloy sets, organized by series.

Sensitivity Analysis: Shadow Prices

The results of a linear optimization problem are a set of decision variables that give the optimal objective function. In the case of secondary alloy production planning, these decision variables are the amounts of scrap and primary raw materials to be purchased. However, linear optimization solutions also provide a powerful set of information that quantifies the sensitivity of these results to changes in assumptions. These sensitivity parameters are known as "shadow prices". Specifically, a shadow price is the change in the objective function at the optimum when a specific constraint is changed by one unit[14] as expressed in Equation (7). Each shadow price has a range of validity associated with it. Interested readers should consult [4, 15] for a lengthier discussion on the value of this information for decision-makers.

$$SP_{\text{Constraint}} = \frac{\delta(\text{Production Cost})}{\delta(\text{Constraint})} \quad (7)$$

Shadow Prices: Composition

As has been shown previously[16], compositional constraints have one of the largest effects on the optimized scrap use and production cost. The magnitude and sign of these shadow prices (derived from Eqs. (5)and (6)) indicates how the production cost would change if the compositional specifications were tightened or loosened. One will notice that shadow prices on the maximum compositional constraints are negative and the shadow prices on the minimum compositional constraints are positive. For example, for alloy 2014, if the constraint on the minimum allowable level of iron were tightened (increased by 1%), the production cost would increase by $144.40. For alloy 4032, if the maximum allowable level of manganese were loosened (raised by one unit), then the production cost would decrease by $276.00. It is no surprise that more of the binding constraints are maximums (28 of the top 50); 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/kiloton) and therefore have the highest impact on the production cost. More interestingly, out of the top fifty largest shadow prices, only ten belong to Set A, the recycling friendly alloys, even though each Set makes up one-third of the total number of compositional constraints. For all compositional specifications, Set A has less constraining compositional specifications than Sets B and C (Figure 2), for example Set A had 25% of its associated shadow prices greater than 10 in absolute magnitude while Set B and C had 39% and 35%, respectively.

Table V shows the shadow prices on the maximum compositional specifications for all three alloy sets for series 4XXX and 5XXX. One can see from the 4XXX series that Alloy C has much higher scrap consumption than its market counterparts 4032 and 4045 because its compositional specifications are much less constraining. Silicon, magnesium, and manganese content is highly constraining for 4032 and 4045 (ie. high shadow prices) while the shadow prices for Scrap C for the same elements are much lower or zero. In contrast, for the 5XXX series, alloy 5052 outperforms Scrap D in scrap consumption and has the lowest shadow price on the most constraining element, iron. One can see that for alloy 5052, the most constraining alloy is shifted to silicon.

The large range in magnitude of these compositional shadow prices indicates that a tool is necessary in order to systematically and efficiently target for development alloys that would provide the most significant improvements in scrap reuse and production cost. The sensitivity analysis results that emerge from this optimization approach provide just this tool.

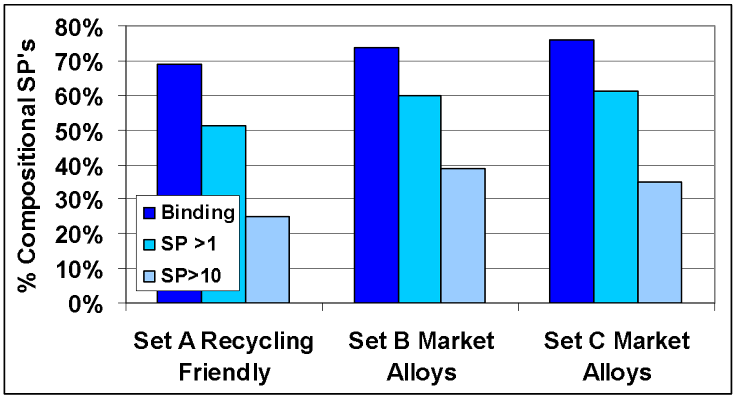

Figure 2. Percentage of compositional shadow prices that are binding, greater than one in absolute magnitude, and greater than ten in absolute magnitude for each of the three alloy sets.

Table V. Shadow prices on maximum compositional specifications for comparison.

Element	C(4XXX)	Alloy 4045	Alloy 4032	D(5XXX)	Alloy 5454	Alloy 5052
Si	0.0	0.9	0.9	1.1	12.1	124.3
Mg	0.0	57.8	34.9	8.6	0.0	0.0
Fe	1.1	2.0	2.0	143.5	146.4	2.0
Cu	13.8	1.5	0.6	0.1	1.2	0.7
Mn	34.0	110.8	276.0	0.0	0.0	72.0
Zn	0.3	15.2	1.2	1.2	1.2	1.2

Conclusions

Despite the fact that the secondary aluminum industry continues to have strong prospects, it, as with any business, must deal with economically significant vagaries in almost every aspect of production. One form of uncertainty peculiar to manufacturing operations is variability in incoming raw materials. This issue is of considerable importance to secondary producers because the very nature of secondary stocks leads to significant variability in quality, including both physical form and chemical composition. The chance-constrained method used for this case study can provide a benefit to producers by allowing statistical information to be embedded into the optimization procedure. This method was successfully used to evaluate scrap consumption of three sets of aluminum alloys. The results of this case study reveal that choosing the portfolio of recycling friendly alloys suggested by Das can enable increased scrap consumption for a typical set of operating conditions. Furthermore, the use of sensitivity analysis from the chance constrained model was shown to be a useful tool to inform decision makers in regards to these strategic alloy choices.

References

1. Das, S.K. *Emerging Trends in Aluminum Recycling: Reasons and Responses*. in *TMS (The Minerals, Metals & Materials Society*. 2006. San Antonio, Texas.

2. Lund, J.R., et al., *Linear Programming for Analysis of Material Recovery Facilities.* Journal of Environmental Engineering, 1994. **120**(5): p. 1082-1094.
3. Stuart, J.A. and Q. Lu, *A Model for Discrete Processing Decisions for Bulk Recycling of Electronics Equipment.* IEEE Transactions on Electronics Packaging Manufacturing, 2000. **23**(4): p. 314-320.
4. Cosquer, A. and R. Kirchain, *Optimizing The Reuse of Light Metals from End-of-Life Vehicles: Lessons from Closed Loop Simulations.* TMS: The Minerals, Metals, and Materials Society, 2003. **AA3**.
5. Shih, J.S. and H.C. Frey, *Coal blending optimization under uncertainty.* European Journal of Operational Research, 1995. **83**: p. 452-465.
6. Gesing, A., et al. *Separation of Wrought Fraction of Aluminum Recovered from Automobile Shredder Scrap*. in *The Minerals, Metals & Materials Society 2001*. 2001.
7. Kattentidt, H.U.R., T.P.R. de Jong, and W.L. Dalmijn, *Multi-sensor identification and sorting of bulk solids.* Control Engineering Practice, 2003. **11**: p. 41-47.
8. Gaustad, G., P. Li, and D.R. Kirchain. *Modeling Methods for Managing Raw Material Compositional Uncertainty in Alloy Production*. in *TMS: The Minerals, Metals, and Materials Society*. 2006. San Antonio, Texas.
9. Charnes, A. and W.W. Cooper, *Chance constrained programming.* Management Science, 1959. **6**: p. 73-89.
10. *EN 13920: Aluminium and Aluminium Alloys-Scrap.* 2003, European Committee for Standardization.
11. Kelly, T., et al., *Historical Statistics for Mineral and Material Commodities in the United States*. 2004, USGS.
12. *Recycling Xchange*. 2006.
13. Gesing, A., *Recycling light metals from end-of-life vehicles.* Journal of Materials, 2001. **53**(11).
14. Neufville, R.d., *Applied Systems Analysis: Engineering Planning and Technology Management*. 1990, New York: McGraw-Hill Publishing Company. 470.
15. Cosquer, A., *Optimizing the Reuse of Light Metals from End-of-Life Vehicles*, in *Engineering Systems Division*. 2003, Massachusetts Institute of Technology: Cambridge, MA. p. 98.
16. Gaustad, G., P. Li, and R. Kirchain. *Managing Raw Materials Compositional Uncertainty: Chance Constrained Modeling for Alloy Production*. in *Materials Science and Technology (MS&T) 2006*. 2006. Cincinnati, OH.