

Toward Sustainable Material Usage: Evaluating the Importance of Market Motivated Agency in Modeling Material Flows

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S Supporting Information

ABSTRACT: Increasing recycling will be a key strategy for moving toward sustainable materials usage. There are many barriers to increasing recycling, including quality issues in the scrap stream. Repeated recycling can compound this problem through the accumulation of tramp elements over time. This paper explores the importance of capturing recycler decision-making in accurately modeling accumulation and the value of technologies intended to mitigate it. A method was developed combining dynamic material flow analysis with allocation of those materials into production portfolios using blending models. Using this methodology, three scrap allocation methods were explored in the context of a case study of aluminum use: scrap pooling, pseudoclosed loop, and market-based. Results from this case analysis suggest that market-driven decisions and upgrading technologies can partially mitigate the negative impact of accumulation on scrap utilization, thereby increasing scrap use and reducing greenhouse gas emissions.

A market-based allocation method for modeling material flows suggests a higher value for upgrading strategies compared to a pseudoclosed loop or pooling allocation method for the scenarios explored.



1. INTRODUCTION

Global consumption of materials has grown exponentially over the last century.¹ In response to that trend as well as threats of stricter regulations and the push for corporate responsibility firms are feeling pressure to move toward creating a more sustainable materials market. One key strategy toward that goal is the increased use of secondary (i.e., scrap or recycled) materials. Increased recycling can forestall the depletion of nonrenewable resources, reduce energy consumption and emissions, and, in many cases, lower the cost of production.²

Given these potential benefits, recycling appears to be a win-win investment. Previous research, however, has raised questions about whether the utility of recycling is ultimately limited by the accumulation of undesirable materials constituents or materials characteristics inherently caused by reprocessing. We propose that current models of materials systems may not accurately reflect the dynamics of accumulation because those models do not explicitly consider the actions of recyclers within the system. Recyclers manage the characteristics of their products and therefore may influence the rate and nature of accumulation. Models that ignore the actions of these agents may not only

misestimate expected accumulation but also undervalue so-called upgrading technologies that mitigate accumulation. Upgrading technologies will not be implemented unless they are economical. Faulty estimates of that value leads to underinvestment in a technology that can improve the sustainability of materials markets. The next sections will provide more detail on the concepts that lead to the formulation of this research and the previous work that guides model development.

1.1. Accumulation and the Role of Agency within a Recycling System. A number of authors^{3–5} have raised concerns that the repeated recycling of a resource degrades that resource, making it increasingly difficult to reuse. This is due to the *accumulation* of certain undesirable elements, compounds, or microstructural changes in the material stream. The mechanisms for accumulation are varied. For many materials, particularly metals, some of these additions are intentional — elements added

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to achieve desired properties. Elements from cutting machinery, typically iron, may be introduced during fabrication, while joining (in the form of welds, rivets, nails, and adhesives) can mix materials as well as impair separation at end-of-life (EoL). Additionally, EoL processing such as crushing, shredding, and paint removal can introduce unwanted elements or microstructural change.⁶

Several studies⁷ have attempted to model the implications of these accumulation mechanisms. One study by Kim et al.,⁵ examining the aging characteristics for recycled aluminum wires, estimates that, even for mixing ratios of primary to secondary materials below 50%, unwanted elements will increase at a steady rate with repeated recycling. Kakudate et al.,⁸ tracking the flow of steel in Japan, estimated that accumulation of Cu will cause a growing amount of steel scrap to become unfit for use; a reduction in recycling rate of 10% is estimated to occur as early as 2020 for contamination ratios greater than 0.4.

Regardless of the mechanism, there are a variety of operational and technological solutions that firms can employ to mitigate the impact of accumulation. Dilution and “down-cycling” strategies, although effective in mitigating accumulation, negatively impact recycling economics through the increased cost of primary additions in the case of dilution, or reduced product value in the case of down-cycling. Other proposed solutions to the accumulation problem are more technically sophisticated and serve to *upgrade* the material, potentially maintaining both economic value and providing environmental benefit. These include strategies such as dismantling of EoL products, spectrographic or magnetic sorting of scrap, and “filtration” technologies that remove elements in the melt such as fractional crystallization and vacuum distillation.^{9–11}

Although these upgrading strategies can improve raw material quality, justifications for investment in their development and deployment depend upon defensible assessments of their economic consequences. These sorts of assessments, however, are challenging. A method that can be used to conduct such an assessment must consistently treat 1) the dynamics of EoL scrap material flows, 2) the impact of flow changes on the economics of production, and 3) the influence of recycling process parameters (e.g., upgrading effectiveness) and recycler decision making (e.g. raw material-to-product allocation) on future accumulation. Previous literature in this area has mainly utilized dynamic material flow analysis (dMFA) methodologies. dMFA methods typically model the reintroduction or reallocation of scraps into a materials production system in one of two ways: a) as a *pooled* scrap stream or b) as a *pseudoclosed loop*. In the pooled approach, scraps are not differentiated by product category and products draw from a common scrap pool. In the pseudoclosed loop approach, scrap is differentiated by product category and categories draw only from their own scrap. Details on the implementation of these methods will be provided in the previous work section.

While the use of models that incorporate these approaches can provide valuable information about the flow of scrap materials, these models fail to fully capture the allocation decisions that are made by market-motivated stakeholders, or agents, within the materials system. This work asks the following questions: Might agent actions alter the rate of accumulation or the implications of that accumulation on potential scrap use? Do modeling methods that capture those agent actions, in turn, differently value potential upgrading technologies that promote increased recycling?

To explore the impact of agent decisions, this work proposes combining dMFA methods with a blending model that minimizes feedstock costs, constrained by the agent’s production goals, to allocate scrap and primary materials to individual product streams. The dMFA methods will enable the model to characterize the composition of EoL scraps. The inclusion of blending models incorporates aspects of agency within the MFA framework, by treating the way that prices lead a recycler to allocate specific raw materials to specific products. This modeling approach is explored in the context of a case study of aluminum use. As a case study, generalized conclusions are inappropriate. Nevertheless, the results presented here suggest that ignoring agents’ economic decisions can lead to faulty estimates of the effects of accumulation, thereby leading to incorrect evaluation of upgrading technologies for mitigating the accumulation effect.

2.0. PREVIOUS WORK

Methodologies for a) tracking material flows and b) modeling allocation decisions both have a rich set of associated literature. Unfortunately, no previous work explicitly explored the effects of accumulation in a multigeneration, multiproduct recycling system.

2.1. Dynamic Material Flow Analysis and Allocation Models. Attaining a sustainable materials market requires understanding the nature and magnitude of the flows within it. A typical material flow analysis is a snapshot of all of the flows of a certain material in a specific region for a set time period. Most MFA research has focused on high volume materials (e.g., iron and steel¹²), high value materials (e.g., silver¹³), or toxic materials (e.g., cadmium¹⁴). To date, most MFA studies have relied upon market-wide statistics that do not capture fine technical structures needed to provide insight into the management of compositional accumulation. For aluminum, the case focus of this paper, published MFA studies are fairly limited, one exception of note is the model created by the International Aluminum Institute (IAI) which has been updated for years 2006 and 2009.¹⁵

A *dynamic* MFA (dMFA) captures the magnitude of material flows over multiple years as well as a projection of future flows by allocating the materials streams according to particular constraints. Two studies of note^{16,17} use a dMFA methodology to examine scrap availability of aluminum over time. These studies detail alloy use by product category. However, as compositional details are not included, this type of modeling implicitly assumes *pooled scrap allocation*. Another pertinent dMFA study comes from Verhoef et al.¹⁸ who developed a complex interlinked model of several metals systems to explore the impact of a transition to lead-free solder on system environmental impact. This study also assumes *pooled allocation*.

Another set of models used to project the availability of recycled scrap streams is residence time models. In these, Markov chain modeling provides estimates of the average number of times an element is used within a materials system. This methodology^{19,20} has been used to estimate characteristics of scrap streams for case studies on steel in Japan⁴ and the United Kingdom,²¹ as well as copper.^{22,23} These studies have focused on how this methodology can overcome allocation issues for life-cycle analysis but not on insights regarding accumulation. In these studies, compositional details are not tracked, and *pooled scrap allocation* is implicitly assumed.

Without compositional details, it is impossible to examine the effects of accumulation. A group at the University of Tokyo

examines accumulation in recycled materials, focusing mainly on steel. This group has examined the accumulation of copper in steel⁸ including the role of exports in that process.²⁴ One article⁴ by this group examines the recycling of aluminum in Japan. In this study, compositional data were collected and aggregated by alloy series, assuming each alloy series composition would equal the average of the maximum specifications for selected alloys within the series. A population balance model was used to project the availability and composition of aluminum scrap out to the year 2050. It was assumed that EoL scrap materials would have a composition equal to the average for its end-use sector. An assumption referred to herein as *pseudoclosed loop scrap allocation*.

2.2. Market-Based Allocation Models. One key aspect of recycling system behavior missing from both static and dynamic MFA is capturing the production decisions that occur at the firm level. Secondary producers are confronted with an array of scrap types from which they decide what to purchase and what to allocate to produce specific alloys, i.e., *market-based scrap allocation*. The producer, therefore, has an important role in determining the actual composition of aluminum material flows.

To guide these decisions, many recyclers use batch-planning tools based on linear optimization techniques,²⁵ a technique that has been applied for decades.²⁶ Because the recycler has direct influence on the composition of their products, they too can influence accumulation. However, of the literature examining blending problems, almost all ignore the passage of time and therefore do not examine accumulation. One exception to this is the body of work by Reuter and van Schaik. This work has been implemented to address recycling policy questions on a large scale in Europe. These studies^{27–29} have used dynamic modeling to guide operational and technological decisions by recyclers and to provide reasonable recovery expectations for the materials system. As the focus of this research has been on automotive recycling, a *pseudoclosed loop scrap allocation* is assumed. However, none of the papers from this group to-date use these models to quantify the degree to which accumulation occurs, how that accumulation is affected by the allocation decisions of recyclers, or how that alters the value of upgrading technologies.

3.0. METHODOLOGY AND CASE DESCRIPTION

3.1. dmFA + Allocation Model. This paper will explore the issues of accumulation, the role of agency, and its impact on the value of upgrading by combining a dmFA model, comprehending the composition of EoL materials, with a material allocation model. Three different material allocation modeling approaches will be compared. These are as follows: 1) *pooled scrap allocation* (Pool) – scraps are commingled and products draw from a common scrap pool; 2) *pseudoclosed loop scrap allocation* (PCL) – scraps are differentiated and products draw only from their own scrap; and 3) *market-based scrap allocation* (MB) – scraps are differentiated and can be used in any product. This model, including all three allocation variants, will be applied to evaluate the impact of accumulation on both recycler economics and potential scrap use.

The dmFA model estimates two basic quantities: the demand for aluminum and the supply of scrap aluminum. To inform the questions surrounding accumulation and upgrading, these quantities are tracked by product sector, by alloy, and with compositional resolution. The demand model is constructed around empirical models of historic and projected production of

aluminum. Formally, aluminum production flows, P , for each year, t , are separately tracked by product sector indexed on $p \in \Phi$ and by alloy, indexed on $j \in J$. Specific models of production flows are described in the Supporting Information (Supplemental A) and take the form $p_{jp} = f(t)$.

The supply model combines three factors to estimate annual scrap collection: historical sales, product lifespan, and EoL collection fractions. Implicit scrap supply flows received, R , for each year, t , are separately tracked by alloy, j , and product sector, p . Implicit scrap availability amounts are calculated using the following relationship

$$R_{jp}(t) = C_p(t) \cdot G_{jp}(t) = C_p(t) \cdot \left(\sum_{s=t^0}^t P_{jp}(s) \cdot \lambda_p(s, t) \right) \quad (1)$$

The mass of scrap (j, p) received in year t , $R_{jp}(t)$, is the amount generated, $G_{jp}(t)$, multiplied times the fraction of EoL products collected in that year, $C_p(t)$. $G_{jp}(t)$ equals the mass of aluminum used in a previous year (indexed on s), $P_{jp}(s)$, multiplied times the fraction of products produced in year s which reached end-of-life in year t , $\lambda_p(s, t)$, summed over all production years prior to t . The actual amount of scrap available, A_i , is determined by the extent to which each allocation approach aggregates incoming implicit scrap streams.

The composition, specifically the concentration of each element, k , of a returning implicit scrap stream, $\hat{\epsilon}_{jpk}(t)$, can be calculated from the composition of the historic alloys of which it is comprised, such that

$$\hat{\epsilon}_{jpk}(t) = \frac{R_{jpk}(t)}{R_{jp}(t)}, \text{ where } R_{jpk}(t) \equiv C_p(t) \cdot \left(\sum_{s=t^0}^t (1 + \alpha_k) \cdot \epsilon_{jpk}(s) \cdot P_{jp}(s) \cdot \lambda_p(s, t) \right) \quad (2)$$

In eq 2, the quantity α_k is the accumulation ratio and is defined as the ratio of the composition of a given scrap to the composition of that aluminum when it was produced. The parameter α will allow the model to test the impact of upgrading (i.e., reducing values of α_k) on system scrap use and economics. The nature and composition of the available scrap (explicit scrap stream, A_i), ϵ_{jpk} , depends upon the allocation strategy.

The actual use and allocation of scrap, while bounded by supply availability, is determined through the use of a simple optimization model. The mathematical details of this model are presented in the Supporting Information, but its basic workings can be described briefly. The allocation model identifies the set of raw materials, scrap and primary, that when combined will produce the desired set of finished goods at lowest cost. Mathematically, this can be represented as

$$x_{ijp}^* = \arg \min_x \{ \text{Cost} | A_I, P_J, \Phi \} \quad (3)$$

where Cost is total cost of raw materials, and x_{ijp}^* is the quantity of raw material i used to produce alloy j for product p . This generalized objective function with constraints tailored by method (Pool, PCL, and MB) enables comparison between the three modeling approaches. Notably, for the Pool and PCL methods, the expression in (3) is equivalent to $\arg \min_x \{ \sum x_{ijp} | A_I, P_J, \Phi \}$, the objective function more commonly found in the literature.

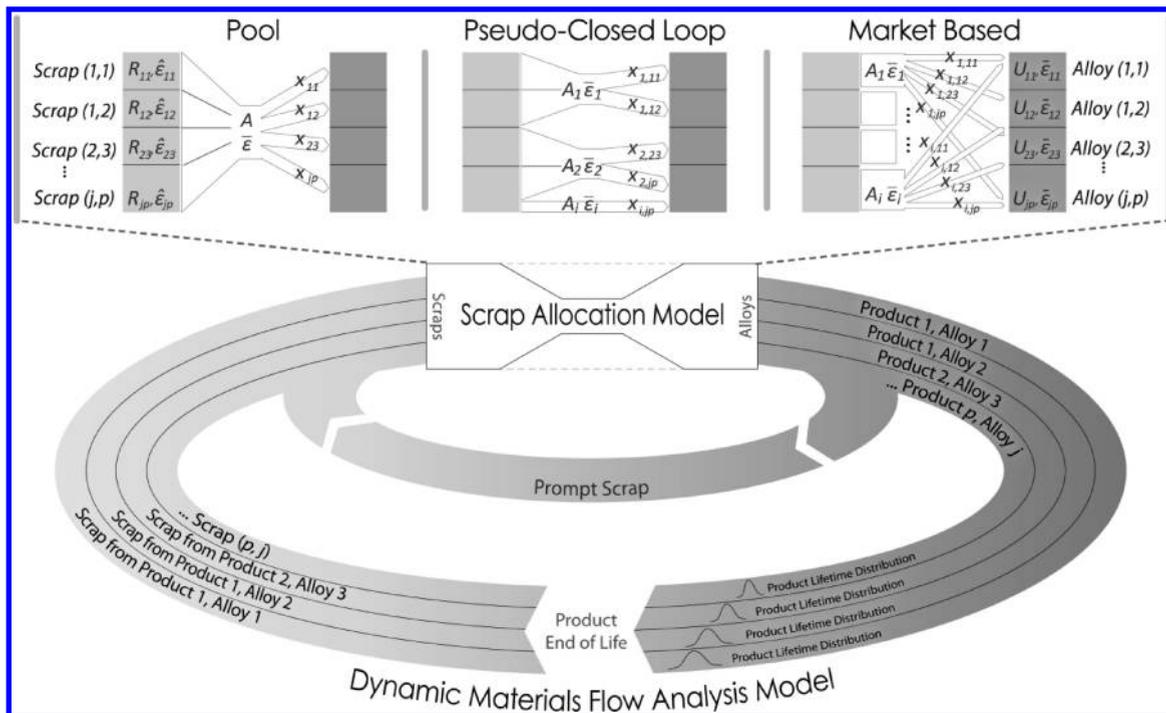


Figure 1. Schematic of dMFA model architecture illustrating the three allocation methods.

Coupling a dMFA and an optimization model of this form represents model architecture similar to that applied by Reuter and van Schaik.²⁸ The inclusion of a market-based model within these allocation strategies provides the capability to capture some of the effects of recycler agency on system behavior. Notably, as applied herein, this still represents a stylized system. The system will be modeled as if only one decision-making agent exists in the market. At every simulated time step, this monopolist has access to all available scraps. Clearly, in a real market there are multiple agents competing for the same sets of scraps. Their access will be limited logistically, and they will therefore make locally optimal decisions that may not align with the overall system optimum. Capturing these behaviors in detail would be expensive in terms of data collection and computational intensity. Nevertheless, the market-based scrap allocation approach serves as a useful extreme test. If this idealization does not lead to significantly different behavior, then the additional analytical effort may be unwarranted for the study of accumulation. Also, the dMFA does not include all streams; for example, the model inputs omit imports/exports. Therefore, the directionality of the results provides the key insights rather than the absolute magnitude of the results. Adding all flows, while informative, would not change the observed trends.

The two models described above work in tandem according to Figure 1. In a given year, the dMFA will provide the availability and composition of specific scraps. The allocation model can then select from these available scraps as well as primary and alloying elements to produce alloys to meet demand for the following year. The resulting production amount as well as the composition of these alloys is then fed back into the dMFA. These products will become scrap material in subsequent years according to their lifetime. More mathematical details are available in the Supporting Information (Supplemental A).

3.1. Examining Accumulation: An Aluminum Case Study. The economic and environmental motivations for recycling are

particularly keen for aluminum. Among bulk metals, aluminum production has one of the largest energy differences between primary and secondary production: 175 MJ/kg for primary compared to 10–20 MJ/kg for secondary³⁰ and has a rapidly growing rate of consumption.³¹ Aluminum also has a large number of problematic accumulating elements in the recycled stream, including both purposefully added and unintended elements accumulating. Much literature exists that pinpoints problematic elements in aluminum including the following: magnesium, nickel, zinc, copper, lead, chromium, vanadium, gallium, manganese, and silicon.^{16,19–21} This combination of characteristics motivates using aluminum as the case material for this paper.

The dMFA + allocation methodology described previously was applied to a case study including the major aluminum industrial sectors (containers and packaging, transportation, and construction). Historical production in the United States from 1975 to 2003 was taken from the United States Geological Survey (USGS) and regressed to create future demand scenarios. A large range in lifetimes was represented, from UBCs in the containers category (less than one year) to siding scrap in the construction category (greater than 45 years). The breakdown in products was chosen to best capture the alloys that make up the majority of returned scrap according to USGS, specifically, UBCs, shredded automotive scrap and castings, and mixed wrought scraps. Further details on this case are provided in the Supporting Information (Supplemental B).

4.0. CASE RESULTS

Before discussing the implications of allocation approach, it is useful to note some gross characteristics of the modeled material flows shown in Figure 2. The largest gains in production are in transportation due to the introduction of more aluminum in the car (for example, in castings, transmissions, and radiators);³² a

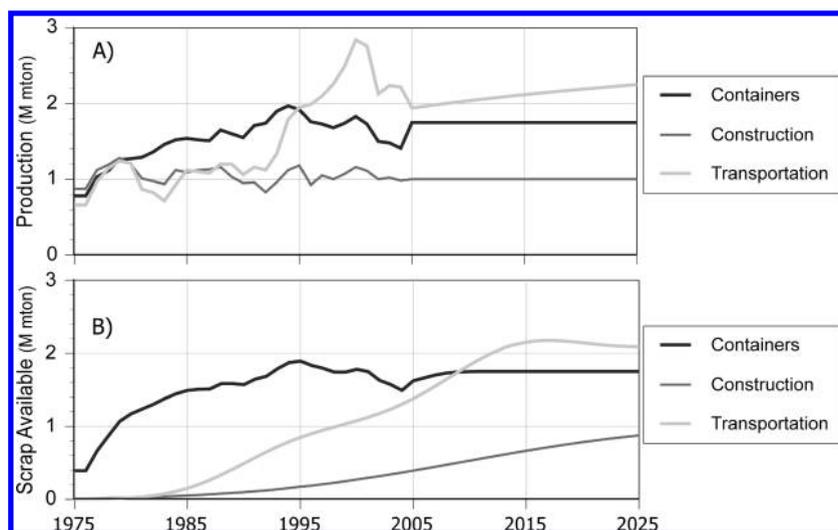


Figure 2. A) Historical production in the US from 1975 to 2006 and projected production trends to 2025. B) Modeled scrap availability in the US for aluminum transportation, construction, and container scrap from average lifetimes. Apparent consumption, as defined by USGS, was used to model the production of aluminum.

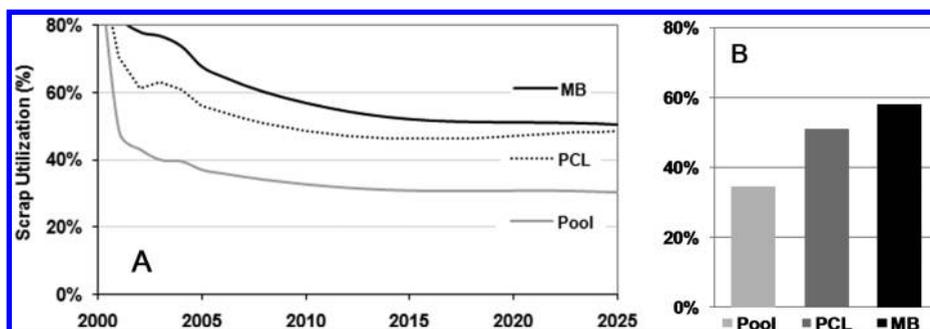


Figure 3. A) Scrap utilization as a percentage of availability by allocation method for each year and B) total scrap utilization over the years 2000–2025 ($\alpha = 1$).

trend expected to continue.^{33,34} Recent historical trends suggest that most other production numbers will plateau (containers, construction, and other). The availability of aluminum scrap is increasing strongly over the modeled time period (Figure 2) particularly until 2015. This is due to both a) increasing overall production in the US over the time frame of 1975–2010 and b) the architecture of the model itself. With regards to model architecture, it takes several years after 1975 to reflect an accurate picture of the returning scrap stream because longer lifetime scraps will not become available for several years. For example, because containers have such a short lifetime, they make up an unrealistic portion of the scrap stream before 1990.

The subsequent analysis will focus on years 2000–2025. Even though availability is increasing, production is also increasing, and the scrap utilization rates become fairly stagnant for years beyond 2010 for all three allocation methods as shown in Figure 3A. Despite similarities in the dynamics, the modeled potential scrap utilization is distinct across the three methods. Modeled scrap utilization remains much higher for both the MB and the PCL methods compared to the Pool method; specifically, MB only drops to a modeled utilization of $\sim 50\%$ compared to Pool which plateaus to a utilization of 30% over the modeled time period. While the PCL method nearly achieves parity at year 2025, the MB method maintains higher modeled usage

throughout the time period modeled (Figure 3B). In reference to the first question this work posed, these results suggest that market-driven stakeholder decisions (i.e., the actions of agents within the system) can alter the impact of accumulation on scrap use. In fact, this result suggests that agent behavior partially mitigates the negative impact of accumulation.

Ultimately, the scrap use associated with each of the allocation approaches derives from the manner in which scrap composition evolves over time. Figure 4 plots the evolution of aggregate composition of three elements over the modeled time period for the three allocation approaches under base case assumptions; this figure makes clear that the allocation approaches differ significantly in the way in which they manage composition. Si appears to become constraining for the Pool method around year 2006 which forces a plateau in composition that the MB and PCL methods do not reach until several years later. Both Cu and Zn have similar trends. For the MB and PCL methods, it appears that Fe and Mn become the constraining elements.

Clearly, both the PCL and MB approaches provide some control over accumulation. For Si (and Cu and Zn), the Pool method creates production strategies that lead to rapid increases in compositions until they constrain further scrap use. Once this occurs, composition slowly declines. In contrast, the PCL and MB approaches prevent rapid accumulation and much more

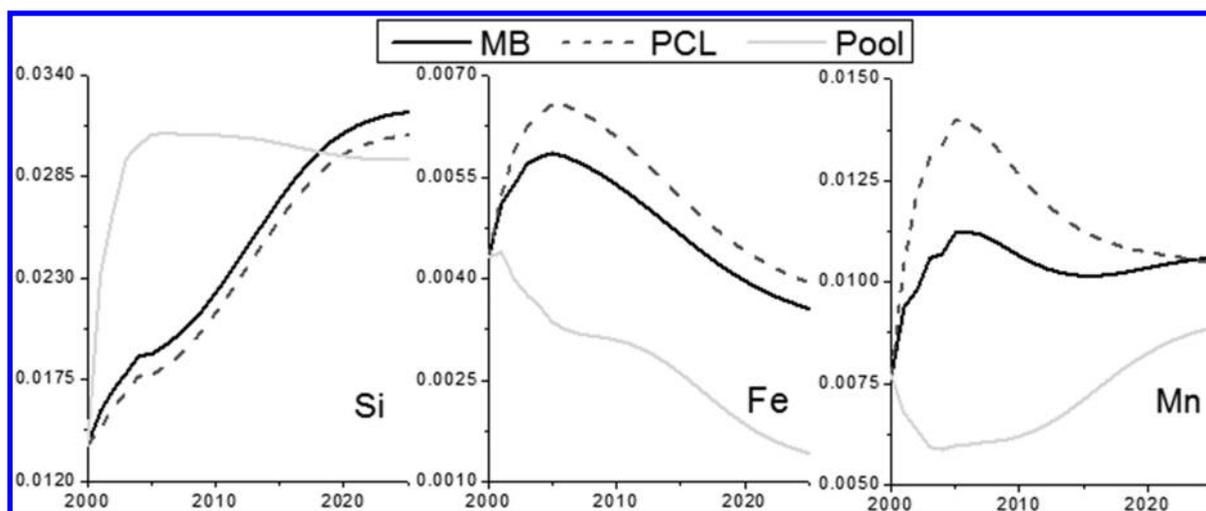


Figure 4. Compositions (in weight fraction) for three tracked elements comparing three allocation methods over time period modeled.

slowly approach the compositional limits (cf. Figure 3B). Here, limits refer to the aggregate maximum and minimum compositional specifications for the portfolio of alloys being produced.

The levels of Fe and Mn behave differently across the three allocation methods. The MB and PCL drive up composition of these elements at a more rapid pace but are able to maintain levels much closer to the limit. Finally, across these elements, the MB method has compositional content between the PCL and Pool methods.

Pooling overestimates the impact of accumulation in an actual scrap stream because it assumes all scraps are being mixed together; this results in more conservative modeled utilization. The PCL model underestimates the degree of accumulation in an actual scrap stream because it assumes that each scrap will be only be used in its same product and thus maintains a homogeneity that does not exist. The MB model projects compositions that lie between these two allocation methods because this method assumes that the scraps can be distributed among the product categories.

This compositional level investigation further emphasizes that market-driven stakeholder actions can alter the rate of accumulation. Furthermore, with the MB method displaying the most moderate (middle) swings in compositions, these results suggest that market-motivated agent actions may in fact mitigate accumulation.

It is also interesting to consider differential scrap use implications across the allocation methods in terms of pressing environmental issues. For example, over the modeled time period there is an 8% difference in potential utilization between the MB and PCL methods (cf. Figure 3B); this represents a difference in modeled scrap used of 240,000 t, all of which would have to be replaced with primary aluminum. Primary production of aluminum has a large environmental burden in terms of global greenhouse gas (GHG) emissions: roughly 15 kg CO₂ equivalents per kilogram of production.³⁵ Thus the scrap difference between the modeled allocation methods would have a large environmental consequence, specifically, 3.6 million kg CO₂ equivalents.

To understand how scrap allocation affects the value of upgrading strategies, it is first useful to understand how allocation and accumulation affect scrap use. The base case assumes an accumulation ratio, α , of 1 and that no explicit approaches (only

allocation) are used to offset accumulation. However, as outlined previously, there are a variety of technological strategies for upgrading scrap currently under development. The degree to which these technologies can successfully mitigate accumulation (i.e., reduce the accumulation ratio) is quite uncertain. As such, rather than explore any one technology, a broad sensitivity analysis around accumulation ratio reduction was performed for all three allocation methods. This allows us to quantify the value of upgrading and compare how that value is affected by the allocation modeling method to address the second question posed by this work.

Figure 5A shows how changes from the base case levels of accumulation rate translate into changes in scrap use for the three allocation methods. One can see that the accumulation ratio has a strong influence on scrap use and, thereby, upgrading could increase scrap use. For the MB allocation method, for example, reducing α by one ($\alpha=0$, $\Delta\alpha=1$) from the base case ($\alpha=1$, $\Delta\alpha=0$), modeled potential scrap use grows by 13 million metric tons, a difference of 25%. The difference in modeled scrap use between the three methods suggests that each method would place a different value on specific upgrading technologies.

Technological upgrading strategies will significantly affect overall emissions as well. Figure 5B shows the corresponding potential reduction in modeled total CO₂ equivalents with increased upgrading for the three allocation methods.

To understand how the allocation strategies differentially value upgrading, an economic analysis offers the critical insight. Figure 6 shows the total production cost savings over time compared to the base case when upgrading technologies are applied to the scrap stream (decreased accumulation ratio). Figure 6A and B show cost savings for two different decreases in accumulation ratio. A ($\Delta\alpha=1$) represents a more effective upgrading technology compared to B ($\Delta\alpha=0.5$). Comparing A to B, not surprisingly, more effective upgrading results in a larger savings in production cost or a higher implied value for upgrading. This is because reducing accumulation allows for increased scrap utilization (cf. Figure 5A). The total value (undiscounted) of these savings is shown in Figure 6C for both levels of upgrading. One can see that the pooling and PCL methods lead to projected costs that imply a lower value for upgrading technologies compared to MB derived results. This is especially

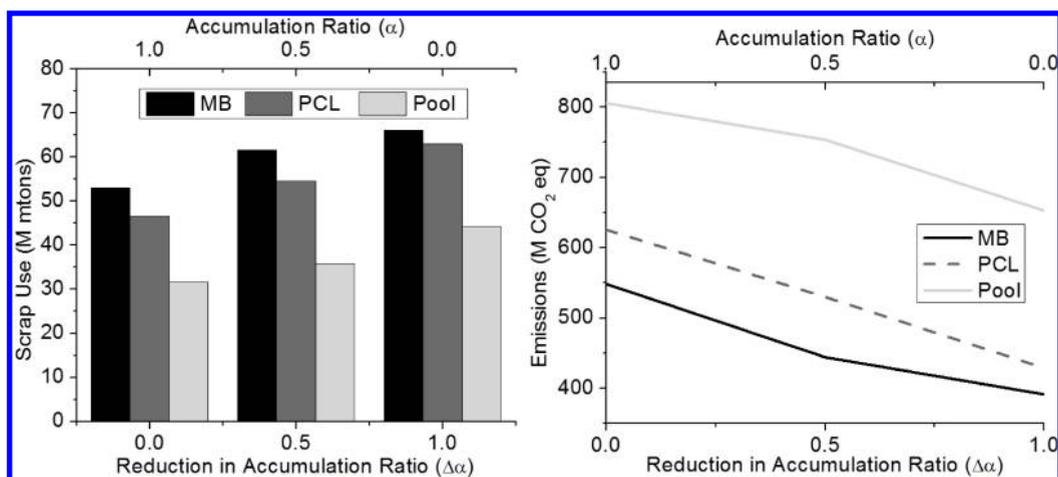


Figure 5. A) Total scrap use comparing the three allocation methods with increasing reduction in accumulation ratio (or increased amount of upgrading) and B) corresponding CO₂ emissions with reduction in α (increased upgrading).

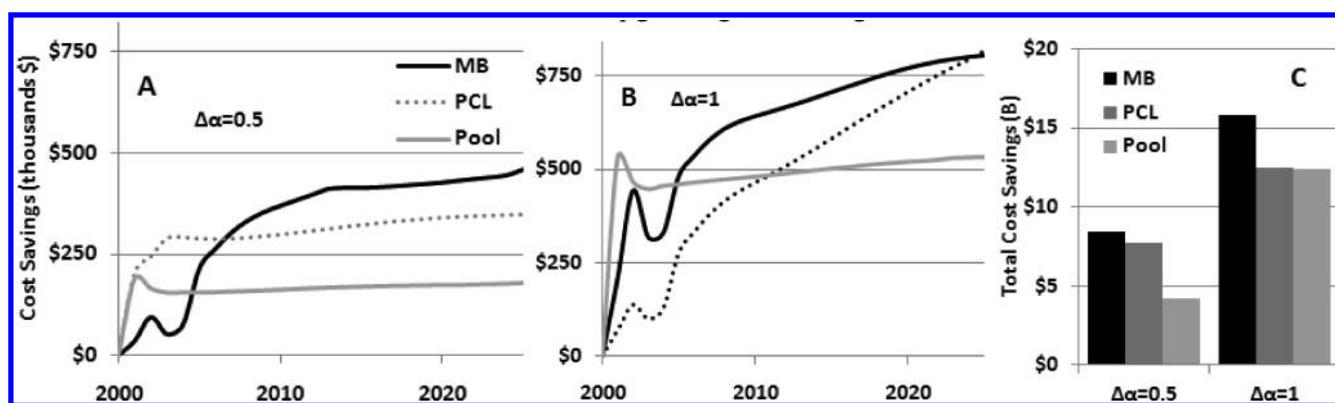


Figure 6. Production cost savings (value of α reduction or upgrading) over modeled time period for market-based blending (MB), pseudoclosed loop (PCL), and pooling (Pool) allocation methods for α reduction = A) $\Delta 0.5$ and B) $\Delta 1$. C) Totals for the entire 25 year span are also shown.

true for the higher difference in accumulation ratio ($\Delta 1$ compared to $\Delta 0.5$). Notably, this analysis considers only cost savings from upgrading. This can be used by firms to perform cost-benefit analysis for a particular upgrading technology with respect to capital equipment and research and development costs. For such assessments, the analysis presented here suggests that the consideration of agency provides a more favorable valuation of upgrading technologies.

Capturing the market-based decisions of agents within models of recycling systems was shown to have a profound influence on modeled scrap use and composition in a case study of aluminum use. In particular, the MB allocation modeling approach was shown to lead to higher modeled potential scrap use (52 million metric tons), followed by the PCL and Pool approaches. These differences in modeled potential usage would translate directly into decreased CO₂ emissions. More critically, accounting for agency within materials systems modeling may more accurately account for the economic value associated with technologies that foster recycling such as scrap upgrading. The MB method projected a much higher value of upgrading as compared to the pooling approach. The results of this paper demonstrate that recycler actions alter the rate and impact of accumulation suggesting that recycler actions can actually mitigate accumulation and increase the ability of a recycling system to maintain high

scrap use. While the case-based nature of this study precludes generalized conclusions, these results provide new appreciation for the actors within a recycling system. The authors hope that this work will also drive the further development of agent-based models of recycling systems, particularly models that account for distributed decision making and supply demand price effects, to ensure that technologies are more appropriately valued and deployed.

■ ASSOCIATED CONTENT

Supporting Information. Supplemental A mathematical model details and supplemental B case details. This material is available free of charge via the Internet at <http://pubs.acs.org>.

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■ REFERENCES

- (1) Matos, G. R.; Wagner, L. *Consumption of Materials in the United States, 1900–1995*; Annual Review of Energy and the Environment, 1998; Vol. 23, pp 107–122.

- (2) Chapman, P. F.; Roberts, F. *Metal Resources and Energy*; Butterworth and Co. Ltd.: London, 1983.
- (3) Daigo, I. Development of a Dynamic Model for Assessing Environmental Impact Associated with Cyclic Use of Steel. *J. Iron Steel Inst. Jpn. (Tetsu-to-Hagane)* **2004**, xxx.
- (4) Hatayama, H.; et al. Dynamic Substance Flow Analysis of Aluminum and Its Alloying Elements. *Mater. Trans.* **2007**, *48* (9), 2518–2524.
- (5) Kim, J.-Y. et al. Aging Characteristics of recycled ACSR wires for distribution lines. In *Electrical Insulation Conference and Electrical Manufacturing & Coil Winding Conference*; Rosemont, IL, 1997.
- (6) Abubakr, S.; Scott, G.; Klungness, J. Fiber fractionation as a method of improving handsheet properties after repeated recycling. *TAPPI J.* **1995**, *38*, 123–126.
- (7) Hatayama, H.; et al. Assessment of the recycling potential of aluminum in Japan, the United States, Europe and China. *Mater. Trans.* **2009**, *50* (3), 650–656.
- (8) Kakudate, K.; Adachi, Y.; Suzuki, T. A macro model for usage and recycling pattern of steel in Japan using the population balance model. *Sci. Technol. Adv. Mater.* **2000**, *1*, 105–116.
- (9) Green, J. A. S. *Aluminum Recycling and Processing for Energy Conservation and Sustainability*; ASM International: Materials Park, OH, 2007; p 267.
- (10) Vigeland, P. Aluminum Recycling: The commercial benefits, the technical issues, and the sustainability imperative. In *Metal Bulletin's 9th International Secondary Conference*; Prague, 2001.
- (11) Veasey, T. J.; Wilson, R. J.; Squires, D. M. *The Physical Separation and Recovery of Metals from Wastes. Process Engineering for the Chemical, Metals and Minerals Industries*; Veasey, T. J., Ed.; Gordon and Beach Science Publishers: Amsterdam, 1993; Vol. I, p 201.
- (12) Wang, T.; Muller, D. B.; Graedel, T. E. Forging the Anthropogenic Iron Cycle. *Environ. Sci. Technol.* **2007**, *41*, 5120–5129.
- (13) Johnson, J.; et al. Contemporary Anthropogenic Silver Cycle: A Multilevel Analysis. *Environ. Sci. Technol.* **2005**, *39*, 4655–4665.
- (14) Hawkins, T. R.; Matthews, H. S.; Hendrickson, C. Closing the Loop on Cadmium: An Assessment of the Material Cycle of Cadmium in the U.S. *Int. J. Life Cycle Assess.* **2006**, *11* (1), 38–48.
- (15) Bertram, M.; Martchek, K. J.; Rombach, G. Material Flow Analysis in the Aluminum Industry. *J. Ind. Ecol.* **2009**, *13* (5), 650–654.
- (16) Boin, U. J. M.; Bertram, M. Melting Standardized Aluminum Scrap: A Mass Balance Model for Europe. *J. Mater.* **2005**, *57* (8), 26–33.
- (17) Martchek, K. J. Material Flow Modeling of Aluminum for Sustainability. In *Aluminum Recycling and Processing for Energy Conservation and Sustainability*; Green, J. A. S., Ed.; ASM International: Materials Park, OH, 2007; pp 103–107.
- (18) Verhoef, E. V.; Dijkema, P. J.; Reuter, M. A. Process knowledge, system dynamics, and metal ecology. *J. Ind. Ecol.* **2004**, *8* (1–2), 23–43.
- (19) Daigo, I. Development of Methodology for Analyzing the Average Number of Times of Use and the Average Residence Time of Iron Element in Society by Applying Markov Chain Model. *J. Iron Steel Inst. Jpn. (Tetsu-to-Hagane)* **2005**, *91* (1), 156–166.
- (20) Yamada, H.; et al. Application of Markov Chain Model to Calculate the Average Number of Times of Use of a Material in Society: An Allocation Methodology for Open-Loop recycling Part 1: Methodology Development. *Int. J. Life Cycle Assess.* **2006**, *11* (5), 354–360.
- (21) Davis, J.; et al. Time-dependent material flow analysis of iron and steel in the UK Part 2. Scrap generation and recycling. *Resour., Conserv. Recycl.* **2007**, *51*, 118–140.
- (22) Eckelman, M. J.; Daigo, I. Markov chain modeling of the global technological lifetime of copper. *Ecol. Econ.* **2008**, *67*, 265–273.
- (23) Giurco, D.; Petrie, J. G. Strategies for reducing the carbon footprint of copper: New technologies, more recycling or demand management?. *Miner. Eng.* **2007**, *20* (9), 842–853.
- (24) Igarashi, Y.; et al. Estimation of the Change in Quality of Domestic Steel Production Affected by Steel Scrap Exports. *ISIJ Int.* **2007**, *47* (5), 753–757.
- (25) Lund, J. R.; et al. Linear Programming for Analysis of Material Recovery Facilities. *J. Environ. Eng.* **1994**, *120* (5), 1082–1094.
- (26) Metzger, R. W.; Schwarzbek, R. A Linear Programming Application to Cupola Charging. *J. Ind. Eng.* **1961**, *12* (2), 87–93.
- (27) van Schaik, A.; Reuter, M. A. The time-varying factors influencing the recycling rate of products. *Resour., Conserv. Recycl.* **2004**, *40*, 301–328.
- (28) van Schaik, A.; et al. Dynamic modelling and optimization of the resource cycle of passenger vehicles. *Miner. Eng.* **2002**, *15*, 1001–1016.
- (29) Reuter, M. A.; et al. Fundamental limits for the recycling of end-of-life vehicles. *Miner. Eng.* **2006**, *19*, 433–449.
- (30) Keoleian, G. A. et al. *Industrial Ecology of the Automobile: A Life Cycle Perspective*; Society of Automotive Engineers, Inc.: Warrendale, PA, 1997; p 148.
- (31) Kelly, T. D.; Matos, G. R. *Historical statistics for mineral and material commodities in the United States*. Aluminum 2010 [cited 2010 7-12-10]. Available from: <http://pubs.usgs.gov/ds/2005/140/> (accessed August 10, 2010).
- (32) Schultz, R. *Aluminum Association Auto and Light Truck Group 2009 Update on Aluminum Content in North American Light Vehicles Phase I*; Ducker Worldwide: Troy, MI, 2008; p 103.
- (33) Gorban, L. T., Ng, G. K.; Tessieri, M. B. An In-Depth Analysis of Automotive Aluminum Recycling in the Year 2010. In *SAE International Congress*; Detroit, MI, 1994.
- (34) Gesing, A. Assuring the Continued Recycling of Light Metals in End-of-Life Vehicles: A Global Perspective. *J. Mater.* **2004**, *56* (8), 18–27.
- (35) McMillan, C.; Keoleian, G. A. Not All Primary Aluminum Is Created Equal: Life Cycle Greenhouse Gas Emissions from 1990 to 2005. *Environ. Sci. Technol.* **2009**, *43* (5), 1571–1577.