Environmental Science & Technology

ARTICLE

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Increasing Secondary and Renewable Material Use: A Chance Constrained Modeling Approach To Manage Feedstock Quality Variation

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S Supporting Information

ABSTRACT: The increased use of secondary (i.e., recycled) and renewable resources will likely be key toward achieving sustainable materials use. Unfortunately, these strategies share a common barrier to economical implementation — increased quality variation compared to their primary and synthetic counterparts. Current deterministic process-planning models overestimate the economic impact of this increased variation. This paper shows that for a range of industries from biomaterials to inorganics, managing variation through a chance-constrained (CC) model enables increased use of such variable raw materials, or heterogeneous feedstocks (hF), over conventional, deterministic models. An abstract, analytical model and a quantitative model applied to an industrial case of aluminum recycling were used to explore the limits and benefits of the CC formulation. The results indicate that the CC solution can reduce cost and increase potential hF use across a broad range of production conditions through raw materials diversification. These benefits increase where the hFs exhibit mean quality performance close to that of the more homogeneous feedstocks (often the primary and synthetic materials) or have large quality variability. In terms of operational context, the relative performance grows as intolerance for batch error increases and as the opportunity to diversify the raw material portfolio increases.

INTRODUCTION

It is estimated that the use of nonfuel materials in the US exceeds 60 kg per person per day.[1] While most of the rest of world uses much less, usage there is growing at twice the rate.[2] Although these estimates are fraught with uncertainty, they point to an emerging global challenge in dealing with the effects of unprecedented levels of materials use. Key strategies that will likely play a role in meeting that challenge are increasing the reliance on both secondary (i.e., recycled) and renewable resources. For recycled resources, energy benefits are well documented and in some cases exceptional.[3] Regarding renewables, the ultimate benefits, which may include reduced energy use, nonrenewable depletion, and carbon burden, remain controversial for many *current* applications. Nevertheless, the trend in renewables technology development is promising.[4] Although rarely discussed together, these two strategies share a common economic barrier to implementation — increased quality variation compared to more conventional resources (i.e., primary mineral ores or synthetics).

The existence of increased variability creates an inherent economic disincentive for using recycled or renewable raw materials. Unfortunately, the most prevalent implementations of batch process planning tools (a key tool for materials producers and recyclers) overestimate this disincentive and thereby undervalue and underutilize such raw materials.

This paper examines the benefits, in terms of cost and variable raw material usage, of one approach to batch planning tools that explicitly considers raw material variability, a chance-constrained (CC) model formulation. Specifically, this paper explores the generality of the benefits of a CC-based model, the drivers of that benefit, and the conditions that maximize benefit.

Before moving to the analysis, the next two sections examine the pervasiveness of quality variability in both recycled and renewable materials contexts and discuss the literature on managing variation in general and, within process industries, on the use of blending models.

Received: October 27, 2010
Accepted: March 22, 2011
Revised: March 7, 2011

EXAMPLES OF VARIATION IN INDUSTRY

Raw material variability confronts many materials producers who use recycled and renewable resources. This section briefly reviews the source of quality variation, the quality performance function (the expression that maps raw material properties to finished good properties) that guides blending decisions, and the methods used currently to accommodate raw material quality variation in examples from four industries.

Inorganics Recycling. Recyclers must manage the quantities of both necessary and undesirable trace elements in incoming feedstocks.[5] For some industries, controlling trace elements provides the greatest technological challenge to expanded recycling.[6] These trace elements are introduced during the recycling process through incomplete separation of components, comingling of end-of-life products or scraps, and processing equipment residue transfer. The stochastic nature of these mechanisms leads to variability in feedstock quality.

Although recent work reports the use of thermodynamic models to quantify the behavior of a metals recycling system,[7] most blending models rely on a performance function that is a linear combination of the constituent feedstocks. Within the recycling industry today, variation is primarily managed through careful selection of suppliers, past experience, and sorting.

Paper. A common challenge across both primary and recycled paper production originates from pulp variability. For primary, significant sources of pulp variation arise from differences in growth habitat and tree age.[8] For recyclate-derived pulp, average fiber length deteriorates with successive use and recycling,[9] leading to variability in quality.

Although multiproperty blending models are a topic of active research, a simple model of paper performance is sufficient to demonstrate applicability of the methods discussed herein. Research has indicated that tear strength is directly proportional to fiber length and that fiber length is a function of the blend of raw materials.[10,11] The existence of such a relationship suggests that a blending model could be implemented to manage feedstock variability.[9,10]

Current strategies to control pulp variation include pulp-property oriented silviculture, the development of proprietary normative blending models, and supplier management.[12]

Rubber. Commercially, rubber is produced from both synthetic materials and natural rubbers. Use of natural rubber remains extensive and is growing as producers seek to increase the use of renewable.[13,14]

The molecular weight of polymer chains in latex, a determinant of rubber properties, differs depending on source location, harvest season, and the extraction process.[15] One of the commercially important characteristics of a rubber precursor is viscosity, a property that is power dependent on molecular weight.[16] A simple blending model for rubber could be based on aggregating the viscosities of constituents according to volume fraction.[14]

Feedstock variation in rubber is managed today through supplier selection, experience-based blending, and preprocessing to modify the average molecular weight of batches.[13]

Collagen and Gelatin. Collagen and its derivative gelatin, two of the most widely utilized bioderived materials, find their way into many applications. The primary feedstocks for collagen and gelatin come from animal sources, although more recently synthetic (recombinant) sources have been developed.

For many applications of collagen, particularly medical uses, the property of interest is solubility, which directly correlates with cross-link density. The cross-link density of collagen varies with the age of the stock and the extraction site.[17,18]

Based on the above performance standards, it should be possible to develop a blending model for collagen based on volume fraction in the blend. For viscosity limited applications, a performance function similar to that for rubber could be applied. For other applications, blend performance is determined by the strength or modulus that scales with the square of the concentration of each constituent.

Commercially, product variability is addressed by maintaining tight control over source-animal history.[19] Additionally, standard collagen and gelatin grades are achieved through experience-based blending.[20]

The examples above suggest that methods to manage feedstock variation could benefit a broad range of disparate industries. As pressure to transition to renewable-based production grows, use of bioderived feedstocks is expected to expand. With this, the need for efficient control of feedstock variation will intensify as well.

A BRIEF REVIEW OF UNCERTAINTY MANAGEMENT IN MATERIALS PRODUCTION

A large body of research has shown that the recycling industries face significant uncertainty in both the quantity and quality of raw materials and, therefore, require particular attention to that issue.[21] In the context of recycling, Guide and van Wassenhove have demonstrated that the stochastic nature of recycled raw materials means that supply chain management is critical to profitability.[21,22] Specific strategies that have been characterized to accommodate and manage feedstock uncertainty for remanufacturers include effective testing and financial incentives,[22,23] careful selection of the mix of products that are remanufactured,[24,25] inventory buffers,[26] and tailored planning models.[27]

Although this literature provides novel insights into strategies to accommodate quality variation, it does so in the context of discrete product manufacturing. Materials production can face a distinct set of challenges.[28] For example, materials can often be produced from a range of recipes that blend feedstocks, as opposed to a fixed bill-of-materials. Manipulating these recipes represents a unique opportunity for managing feedstock quality.

Optimal blending models have been a topic of study for more than six decades. The most common approach involves the use of linear programming to identify the lowest-cost mix of raw materials to yield an end product of given specifications.[29,30] These linear formulations are pervasive in industry and the literature, including examples concerning petrochemicals,[31,32] agricultural products,[33] and recycling.[34,35] More recently, such models have been modified to include thermodynamic-based performance functions.[7,36] Although powerful, each of these models treats the raw material quality as deterministic and known.

Some authors have explored strategies to address feedstock uncertainty. In fact, Debeau warned about this challenge in 1957.[37] This work led to the development of strategies that incorporate information about feedstock quality variation within a linear performance constraint.[38−41] As will be detailed subsequently, although these approaches do improve the robustness of the batch plan, they do not completely characterize how variation manifests in the resulting batch. Another strategy described in the literature uses linear performance constraints (generally based on the mean quality of feedstocks) but manages variability with a penalty function in the objective.[42−44] The relative performance of these methods is beyond the scope of this work.

A final set of literature utilizes a chance-constrained, CC, formulation of the performance constraints to more explicitly model the implications of feedstock variation. CC variants were first formulated by Charnes and Cooper.[45] This technique has found several applications in problems such as feed mixing,[46] materials production,[34,47,48] and coal blending.[49] This set of literature has demonstrated the potential benefits of the CC-formulation through numerical experiments around specific cases. However, to date, there has been no analytic characterization of the benefit of using a CC formulation as compared to one with a linearized constraint.

This paper will address this gap by demonstrating three concepts: i) raw material diversification as the fundamental mechanism for a CC formulation to reduce cost and increase variable raw material usage; ii) the generality of that improvement for materials production where performance is proportional to the performance of the constituent raw materials; and iii) the properties of both raw materials and the operational context that will maximize the benefit of the CC programming method. Together these demonstrations should help to identify the most promising contexts where this modeling approach can improve our ability to use secondary and renewable resources. To explore these issues, this paper compares examples of a conventional deterministic model to a CC-based model. These methods are compared analytically and through a simplified quantitative case analysis in terms of cost and potential variable raw materials usage.

■ FRAMING RAW MATERIALS QUALITY UNCERTAINTY AT THE MATERIALS PROCESSOR

To understand the implications of the two modeling approaches, an uncertainty-aware model was conceived and compared to a conventional model used in the materials industry. The models were built around a case where a materials producer (Producer), attempting to minimize cost, purchases and blends multiple feedstocks to generate finished goods that meet given quality specifications. Feedstocks consist of those with known, certain composition referred to as homogeneous or uniform feedstocks (uF) representing primary/synthetic materials and those with different, uncertain composition referred to as heterogeneous feedstocks (hF) representing secondary/renewable materials. When the blending decision must be made, the exact quality of the feedstock is unknown, but that quality is characterized by a known distribution. The Producer must decide what quantity of each feedstock should be blended in the production batch.

■ MODEL FORMULATION

General Assumptions. One simplified instance of the above scenario involves a Producer who manufacturers one finished good by blending feedstocks, indexed by $i = (0,...,N)$ into a final product. The feedstocks have price ψ_i and quality that varies normally$\sim(\varepsilon_i,\ \sigma_i^2)$. This simplified problem includes one uF $\sim(\sigma_0^2 \equiv 0)$ and two hFs. Only a single generic maximum performance metric given by ε_x will be examined, but analogous conclusions can be derived for a minimum performance metric. Two reduced variables are used to simplify the solution: $E_i = (\varepsilon_i - \varepsilon_0)$, a variable that describes the *quality divergence* of hF_i from the uF, and, $P_i = (\psi_i - \psi_0)$, a variable that describes the *price reduction* of hF_i from the uF. Given that the scenario of interest is when the hFs are less expensive than the uF, P_i, the price reduction, is assumed to be a negative number (each ψ_i is positive). Similarly, the case of interest is when the hFs have a mean performance metric above the uF (i.e., they are further from the maximum specification than the uF). As such, the sign on E_i is positive.

Conventional Linear Risk Formulation. Single metric models (e.g., mean quality performance) and models that address uncertainty by setting the quality specifications to more stringent limits are prevalent in the literature and practice. However, neither of these approaches provides an endogenous mechanism to characterize variability that is sensitive to the characteristics of the feedstocks. As such, the conventional model developed herein makes the frequency that the batch plan is out of specification a function of the feedstock properties. This can be accomplished by representing the feedstock in terms of a range of expected composition, $\{\varepsilon_i \pm B\sigma_i\}$, where B (a non-negative number) determines the amount of variation taken into account when satisfying the performance constraint.[39,43,44] The magnitude of $B\sigma$ affects the likelihood that the finished good quality lies outside of the given specifications.

This conventional approach to framing constraints by a range on expected feedstock composition combined with the notation above leads to a formulation that will be referred to as a deterministic or linear risk (LR) model (for problems bound by a maximum constraint)

$$\text{Min}: C = \Psi_0 + \sum_{i=1}^{N} x_i P_i \tag{1}$$

$$\text{Subject to}: \varepsilon_0 + \sum_{i=1}^{N} x_i E_i + B \sum_{i=1}^{N} x_i \sigma_i \leq \varepsilon_x \tag{2}$$

$$\sum_{i=0}^{N} x_i = 1; 0 \leq x_i \leq 1 \tag{3}$$

where x_i is the fraction of the final product made of feedstock i. Equation 2 is the compositional performance constraint. Equation 3 ensures conservation of mass. A constraint on non-negativity is also required. Notably, both this formulation and the CC formulation explored subsequently comprehend only the costs of raw materials. For many basic materials industries this represents the vast majority of total operating costs.

A particular advantage of the simplified formulation is that it places both the objective function 1 and primary constraint 2 into two dimensions, allowing graphical exploration. Based on the positive signs of E, B, and σ and the negative sign on P described above, the constraint defines a feasible region (shown in white in Figure 1a and b), beyond which the finished good is out of specification. The optimum, $\{x_i^{*,LR}\}$, occurs where the lowest cost isoquant touches the constraint space. This figure indicates that, unless the cost function is parallel to the constraint line (in which case the optima is

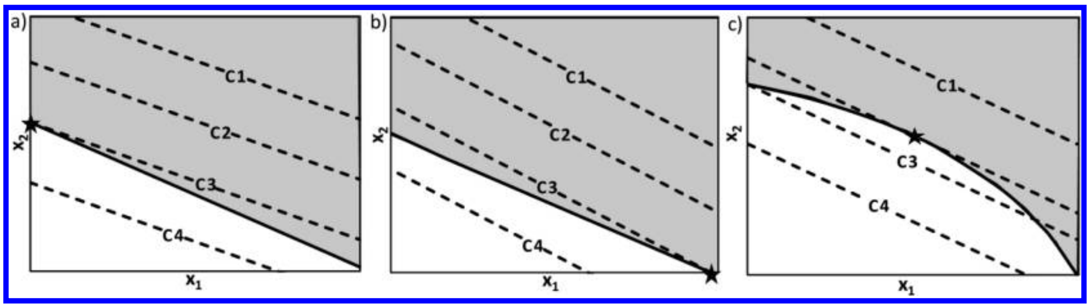

Figure 1. a) and b) Graphical representation of the two common solutions to the LR model. c) Graphical representation of the common solution to the CC model. C4 > C3 > C2 > C1. The star indicates the optimum.

ambiguous), the optimal solution will lie at an axis intercept, leading to the solutions

$$x_1^{*,LR} = 0, x_2^{*,LR} = \frac{\varepsilon_x - \varepsilon_0}{E_2 + B\sigma_2}, \text{where } \frac{P_1}{P_2} < \frac{E_1 + B\sigma_1}{E_2 + B\sigma_2} \text{ or } \frac{P_1}{E_1 + B\sigma_1} > \frac{P_2}{E_2 + B\sigma_2}$$
$$x_1^{*,LR} = \frac{\varepsilon_x - \varepsilon_0}{E_1 + B\sigma_1} x_2^{*,LR} = 0, \text{where } \frac{P_1}{P_2} < \frac{E_1 + B\sigma_1}{E_2 + B\sigma_2} \text{ or } \frac{P_1}{E_1 + B\sigma_1} > \frac{P_2}{E_2 + B\sigma_2} \tag{4}$$

Clearly, cases could exist (e.g., E is small), where the compositional constraint is not binding and $x_i^{*,LR}$ takes the value of one (i.e., the finished good comprises only hF). These cases are not of practical interest.

Two insights emerge from this result. First, a formulation that describes the variance as a linear blend will generally result in a solution where one of the two hFs is not used. Second, this condition is not true (and the solution has alternative optima) when the feedstocks are equivalent in terms of the price reduction per unit of risk-adjusted ($B\sigma$) quality divergence, ($P/(E+B\sigma)$).

Although this form of batch planning model is prevalent,[28] it underperforms other formulations.[34,49] The next section will explore the drivers of this underperformance.

Chance-Constrained Formulation. In the context of batch planning, the chance-constrained method modifies the quality constraints such that solutions provide a specified level of confidence, α, for meeting specifications. Using this approach for the problem at hand, the model formulation retains eqs 1 and 3, but the quality constraint (eq 2) becomes

$$\Pr\{\varepsilon_0 + \sum_{i=1}^{N} x_i E_i \le \varepsilon_x\} \ge \alpha \Rightarrow \varepsilon_0 + \sum_{i=1}^{N} x_i E_i + \Phi(\alpha)\sqrt{\sum_{i=1}^{N}\sum_{l=1}^{N} \rho_{il}\sigma_i\sigma_l x_i x_l} \le \varepsilon_x \tag{5}$$

which reduces to the following when the feedstocks are uncorrelated

$$\varepsilon_0 + \sum_{i=1}^{N} x_i E_i + \Phi(\alpha)\sqrt{\sum_{i=0}^{N} x_1^2\sigma_1^2} \le \varepsilon_x \tag{6}$$

In both of the above, $\Phi(\alpha)$ is the inverse of the normalized cumulative Gaussian distribution function, and ρ_{il} is the correlation between the quality of feedstock i and l. ($\rho_{il} \equiv 1$ when $i = l$.)

Before exploring the analytical solution to the CC formulation (details of which are presented in the Supporting Information), it is first useful to examine the geometry of the problem. As shown in Figure 1c, the solution space is circumscribed by a unique ellipse, defined by eq 6, along which the *risk* of not meeting the constraint is *constant*. As before, the constraint defines a feasible region (white) beyond which the finished good is out of specification. From the geometry, it is clear that, unless the cost function is either exceptionally steep or shallow, the optimum will occur away from the axes. In contrast, the LR solution occurred at the axes, with only one nonzero hF. For the CC formulation, the optimal batch plan diversifies by, generally, containing both of the hFs.

Exploring the Benefit of CC Formulation - Solution Analysis. The usefulness of developing analytical solutions to the two formulations derives from their comparison. This section will compare the resulting batch plans in terms of both cost and the amount of hFs that can be accommodated for an equivalent level of risk of being out of specification − the batch failure rate.

The first question that warrants exploration is the comparability of the batch failure rates of the two formulations. In the case of the CC solution, $\Phi(\alpha)$ explicitly captures failure rate. While the LR model uses an analogous term in its formulation, B, it does not directly translate into any conventional statistical characteristic. Comparing the compositional constraints of the two formulations (i.e., eqs 2 and 6), the constraints converge, when x_1 or x_2 equals zero. As such, the constraints share common intercepts and, therefore, represent the same level of risk at these points. Because the LR model generally leads to a solution only at these points, the optima of both formulations have the same risk and $B = \Phi(\alpha)$ for most optima.

Moving back to the performance of the two solutions, the geometry of the problem demonstrates that the CC formulation will generate batch plans of lower cost. If one requires that the comparable LR case must have the same error rate as the CC solution, then both solutions lie on the same ellipse (See Figure 1.). The LR solution will be on one of the two axes; the CC solution at the point of iso-cost tangency. Unless that point of tangency occurs at an intercept, the CC solution will always be above the iso-cost line intersecting the LR solution, leading to a lower cost for the CC solution.

To understand the range of applicability of these conditions, it is necessary to characterize what conditions would lead the CC solution to fall at an intercept and, therefore, offer no benefit. This would occur when the slope of the iso-cost line is tangent to the ellipse at x_1 or $x_2 = 0$. The conditions for this can be developed from eqs 1 and 6 as

$$-\frac{p_1}{P_2} = \left.\frac{\partial(\Phi(\alpha)\Xi - \Lambda)}{\partial x_1}\right|_{x_1=0} = -\frac{E_1}{E_2 + \Phi(\alpha)\sigma_2} \text{ and } -\frac{P_2}{P_1} = \left.\frac{\partial(\Phi(\alpha)\Xi - \Lambda)}{\partial x_2}\right|_{x_2=0} = -\frac{E_2}{E_1 + \Phi(\alpha)\sigma_1} \tag{7}$$

dx.doi.org/10.1021/es103486s |*Environ. Sci. Technol.* XXXX, XXX, 000–000

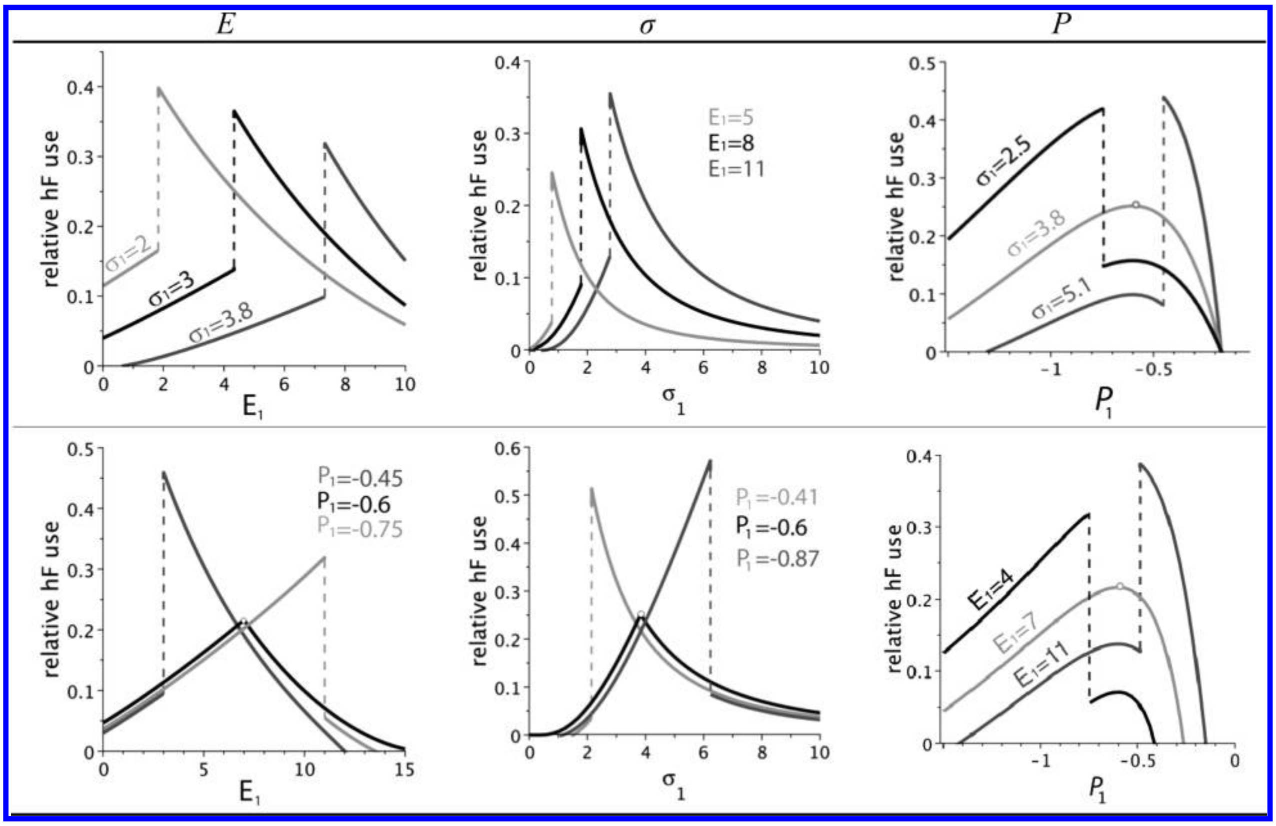

Figure 2. Relative hF use (R) for three parameters of interest: E, σ, and P. Each column shows a family of R curves holding one parameter constant. For example, the top left plot demonstrates the change in E_1 at various values of σ_1 holding P_1 constant. Values unless otherwise noted: $E_1 = 4.5$, $\sigma_1 = 3$, $E_2 = 5.5$, $\sigma_2 = 3.5$, $\varepsilon_x = 40$, $\varepsilon_0 = 36$, $\Phi(\alpha) = 3$, $P_1 = -0.5$, $P_2 = -0.6$, $\psi_0 = 1.5$.

where $\Phi(\alpha)\Xi - \Lambda = \varepsilon_0 + \Sigma_{i=1}^{N} x_i E_i + \Phi(\alpha)(\Sigma_{i=1}^{N} x_i^2 \sigma_i^2)^{1/2}$. Rearranging these for a parameter of interest describes the range of conditions where the CC solution offers benefit. Thinking of these boundaries in terms of a hypothetical example provides some insight into their physical meaning. Considering a case where the second feedstock appears less desirable due to a higher quality divergence, $E_2 > E_1$, the following question arises: under what conditions would the solution include the lesser feedstock in the batch plan. This condition can be identified specifically by rearranging the condition described in eq 7 and comparing this to the LR condition described by eq 4 (both are shown in eq 8). From this, we see that the criterion for $x_2 \neq 0$ for the LR solution is more stringent than for the CC formulation. This means that using a CC-based model, apparently less-desirable raw materials (x_2 in this case) are used in the batch plan across a broader range of prices, mean quality, and quality variability than in a LR-based model

$$\text{CC condition for } x_2 \neq 0; \frac{P_2}{E_2} < \frac{P_1}{E_1 + \Phi(\alpha)\sigma_1}$$
$$\text{LR condition for } x_2 \neq 0; \frac{P_2}{E_2 + \Phi(\alpha)\sigma_2} < \frac{P_2}{E_1 + \Phi(\alpha)\sigma_1} \quad (8)$$

Insights into relative hF use between the models can be gained from a combined quantitative assessment and analytical solution. Figure 2 plots the difference in hF use between the solutions, R, defined as

$$R \equiv \frac{(x_1^{*,CC} + x_2^{*,CC}) - (x_1^{*,LR} + x_2^{*,LR})}{(x_1^{*,LR} + x_2^{*,LR})} \quad (9)$$

for a comprehensive set of problem characteristics. Each column in the figure plots R for a range of one characteristic (e.g., E) for six combinations of the other two parameters (e.g., σ and P). Notably, each plot displays a maximum for R, generally a marked, discontinuous maximum. In all cases, this maximum occurs at the indeterminate point for the LR optimum. As shown in eq 4, this occurs when $(E_2+B\sigma_2)/P_2 = (E_1+B\sigma_1)/P_1$. One way of interpreting this criterion is that the gain from the CC solution is maximized when the hFs are "equivalent" from the perspective of their relative effect on cost. As such, one attribute of a case that will maximize the benefit of the chance-constrained formulation arises when the hFs are similar. Exploring this particular point of the solution space illustrates which characteristics increase the CC benefit.

An obvious example that meets the conditions of scrap equivalence occurs when the hFs in fact share the same characteristics, such that $P_1 = P_2 = P$; $E_1 = E_2 = E$; and $\sigma_1 = \sigma_2 = \sigma$. For these conditions, the solutions shown in the Supporting Information reduce to

$$x_1^{*,CC} = x_2^{*,CC} = \frac{\sqrt{2}}{2} \frac{(\varepsilon_x - \varepsilon_0)(\Phi(\alpha)\sigma - \sqrt{2}E)}{\Phi(\alpha)^2\sigma^2 - 2E^2} \quad (10)$$

Comparing this to the level of scrap used in the LR solution (i.e., eq 4) yields the result for two hFs as well as an arbitrary

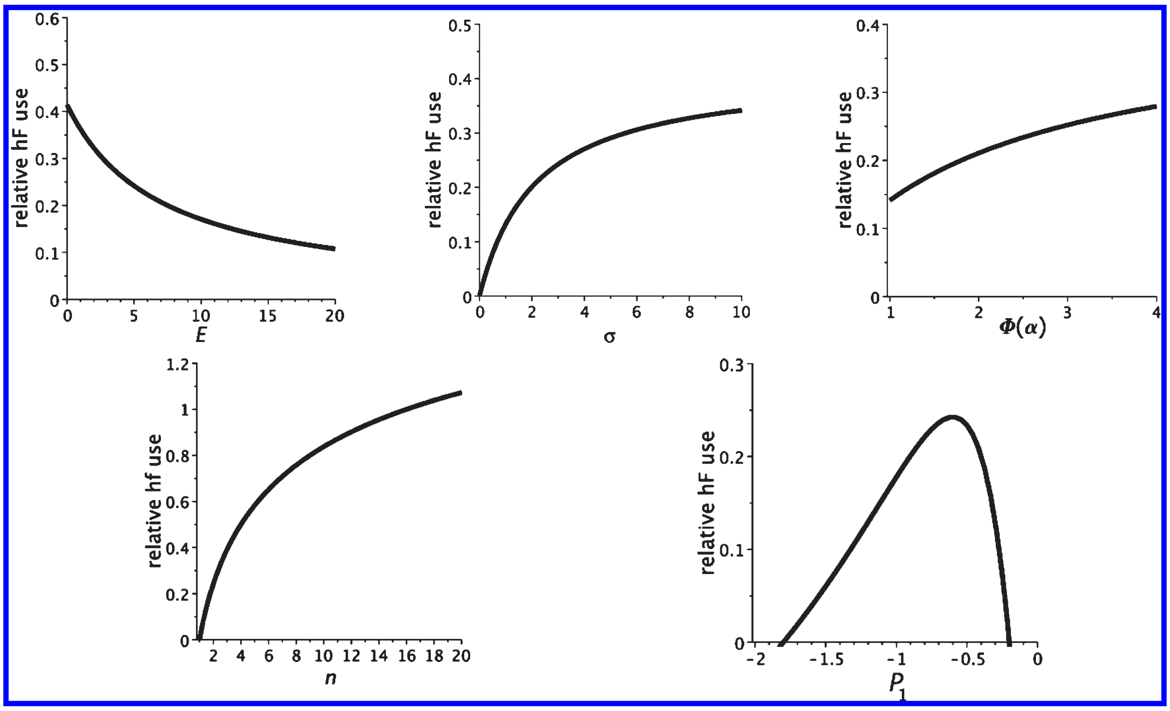

Figure 3. Relative hF use (R) for stylized solution given in eq 11 for parameters, E, σ, $\Phi(\alpha)$, n, and P, showing the partial derivative of R in terms of each parameter. Values used: $E/E_1 = 4.5$, $\sigma/\sigma_1 = 3$, $n = 2$, $E_2 = 5.5$, $\sigma_2 = 3.5$, $P_2 = -0.6$. Corresponding mathematical solutions are provided in the Supporting Information.

number, n, hFs

$$R = \frac{((\sqrt{2}-2)E + (\sqrt{2}-1)\Phi(\alpha)\sigma)|\Phi(\alpha)\sigma|}{\Phi(\alpha)^2\sigma^2 - 2E^2} \Rightarrow \frac{(\sqrt{2}-1)\Phi(\alpha)\sigma}{(\Phi(\alpha)\sigma + \sqrt{2}E)} \Rightarrow \frac{(\sqrt{n}-1)\Phi(\alpha)\sigma}{(\Phi(\alpha)\sigma + \sqrt{n}E)} \qquad (11)$$

Given the nature of the parameters, these expressions will always be positive for $n \geq 2$, indicating that the CC formulation will always increase hF use when more than one hF is available and the compositional constraint is binding.

The results in eq 11 indicate what characteristics of a specific case amplify or diminish the CC-associated benefit. Examining the partial derivatives of R provides one method to explore this benefit. Figure 3 summarizes the nonzero derivatives for R. These results suggest that the relative benefit of the CC method should *decrease* asymptotically as E grows, while it should *increase* asymptotically as σ, $\Phi(\alpha)$, or n grow. The relationship in eq 11 is also informative insofar as what is absent. Specifically, we could infer that neither ε_0 nor ε_x influence the relative difference in hF use.

In order to investigate the final parameter, price, it is necessary to return to the more general solution. The last figure of Figure 3 shows the partial derivative for R in terms of P_1 for the general solution without common parameters. (The result for P_2 is comparable.) Within the range of validity for the CC solution, all of the terms in this equation will maintain a consistent sign as price is varied, with the exception of the first, $(P_1 - P_2)$. As such, the benefit reaches a maximum when the prices are the same. As price moves away from this point, the CC benefit declines as one hF becomes the dominant constituent within the batch plan.

This analysis would suggest that the CC formulation always performs equal to or better than the LR formulation and that there are conditions where a CC formulation would lead to both increased use of heterogeneous feedstocks and lower production costs. The value of these results derives from whether they adequately represent the type of behavior displayed in a more realistic case. The following quantitative example approximates the scope of a real production situation and has been based on actual industry data for a particular metal recycling firm. Further case specific observations and analyses on the benefits of a CC formulation related to recycling within the aluminum industry can be found in previous work by the authors.[34]

■ CASE EXAMPLE: ILLUSTRATING THE BENEFIT AND LIMITS OF THE BENEFIT IN THE CONTEXT OF ALUMINUM RECYCLING

Real production cases are far more complex than the analysis developed above. As such, this section explores the performance of scalable versions of a linear-risk based and chance-constrained based batch planning model in the context of a real-world case of aluminum recycling. For this case, the models examine the problem of mixing quantities of up to fifteen feedstocks, up to eight of which are scraps, all of unlimited availability, to produce an identical mass of two finished goods at lowest cost. The LR model was formulated according to eqs 1, 2, and 3. The CC model was formulated according to eqs 1, 2, and 6. Both were executed using a global, linear/nonlinear programming optimization engine. The case selected for this study represents the production decisions of a North American aluminum recycler that produces a broad range of alloys including the two finished goods being modeled. The scraps represent raw materials that were available and used by that producer during 2008. The quality measure for this case is the composition of the scrap materials and the finished goods into which they are blended.

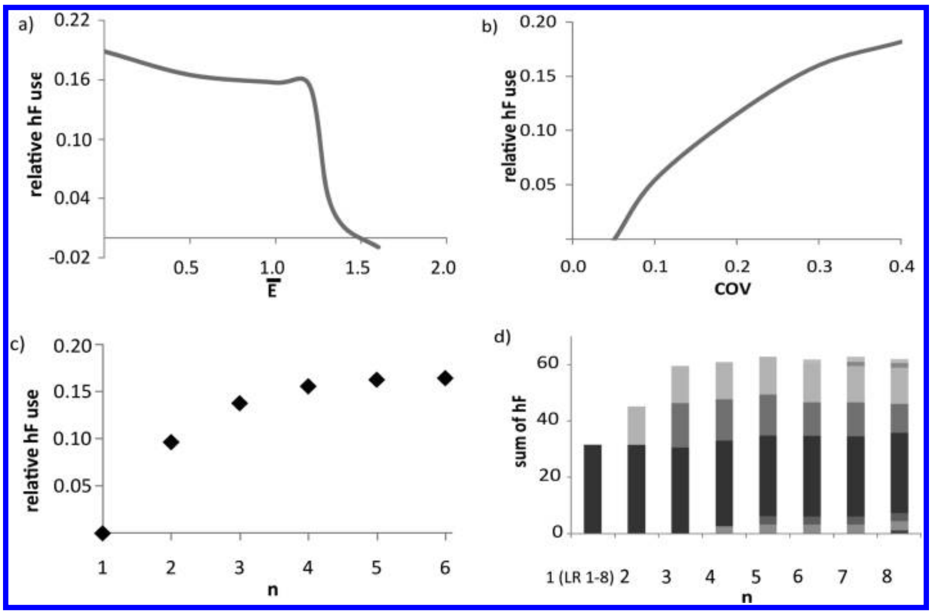

Figure 4. a) − c) *R* versus *E*, COV, and *n* and d) the hFs used in the solution for the both the LR and CC solution for $n = 1-8$.

Composition is tracked using six trace elements (Cu, Fe, Mg, Mn, Si, and Zn). In the terminology of the analytical model the scraps are hFs with higher quality variation. The uFs comprise a primary aluminum feedstock and pure feedstocks for each of the alloying elements, all of narrow quality variation.

Figure 4a-c plots *R* (as defined in eq 9) based on the results of both the LR and CC models. Specifically, the plots in Figure 4a-c show *R* for changes in a) *E* (for the base coefficient of variation, or COV, of 40%), where COV $\equiv \sigma_i/\varepsilon_i$ or the ratio between standard deviation and mean, b) COV, and c) *n* (number of available hFs), respectively. *E* describes the fraction that the hFs are above the original specification. Variation in terms of COV was included here as a way to explore the implications of relaxing the assumption of constant variation (i.e., constant σ).

It is apparent from comparing the graphs shown in Figure 4 with those in Figure 3 that *R* exhibits similar behavior to that deduced from the analytical solution. This means that the relative benefit of the CC method should decrease asymptotically as *E* grows and increase asymptotically as σ and *n* grow. The plot of *E* differs slightly from the analytical version shown in Figure 3. For the aluminum recycler case, there are two distinct regions of asymptotic decline. This occurs because as *E* grows, the solution space shifts from one set of binding compositional constraints to another. The second difference between Figure 4a and the analytical solution occurs at high values of *E*. In the limit of *E*, the CC solution no longer outperforms the LR in terms of scrap use. This results from the fact that the optimization formulation minimizes cost rather than maximizing scrap use. At high values of *E*, the hFs provide more value to replace the alloying elements rather than the base metal; therefore, the amount of potential hF usage is lower. These observations indicate that the CC solution provides more benefit when the hFs exhibit mean quality close to that of the uFs, where quality variability is large and where the number of available hFs is high. The behavior observed regarding quality variability is consistent with case specific observations made by others applying the CC approach to cases of steel, coal, and aluminum blending.[34,48,49]

The most fundamental observation concerning the behavior of the CC formulation comes from examining how the batch plans for the CC and LR solutions change with *n*, the number of available hFs. The first insight on this issue emerges from the earlier geometric analyses, which indicated that the LR model will generally identify batch plans with only one hF, while CC-derived batch plans would incorporate multiple hFs. Figure 4d shows how the batch plans for the case analysis respond to changes in *n* for one to eight available hFs. Notably, the intuition of the two hF analytical solution holds − the CC model constructs batch plans comprising larger numbers of raw materials. It is this behavior that is the ultimate driver of benefit for the CC model. By constructing a batch plan using a portfolio of feedstocks, the CC method manages variation, while increasing hF use.

Increasing the use of secondary and renewable raw materials will likely be an important part of the shift to sustainable production. Based on these analyses, it is clear that there are likely cases where materials producers could manage their quality uncertainty while still using more of these raw materials than a conventional analysis would suggest. This increase in heterogeneous raw materials usage seems counterintuitive: how could one increase the variation while still meeting performance specifications? This analysis has shown that this is possible because a CC model formulation identifies portfolios of raw materials whose uncertainty characteristics are superior to that of any individual raw material. By creating a portfolio of raw materials, it is possible to manage risk and cost simultaneously. These observations are analogous to ones made in early study of risk-constrained financial portfolio theory[50] but cannot be derived directly from that work due to differences in the objective function and performance constraints across the two cases.

The gain from the CC formulation is strongly influenced by characteristics of both the available raw materials and the operational context. Overall, the results indicate that the CC solution will provide more benefit for cases where the heterogeneous raw materials are similar in their characteristics, where the heterogeneous raw materials exhibit mean quality performance close to that of the homogeneous analogs (*E* and ΔE are small) and where variability is large (σ or COV is large). In terms of operational context, the relative performance of CC-based batch plans grows as concern over batch error grows (Pr{batch error} is small or $\Phi(\alpha)$ is large) and as the opportunity to diversify the raw material portfolio increases (n is large).

Ultimately, to realize the benefits discussed in this paper, materials producers will need to both collect information on raw material quality and develop reasonable models of blend performance. Nevertheless, armed with appropriate decision-support models, materials decision makers should be able to improve the economic and environmental performance of emerging sustainable materials technologies.

■ ASSOCIATED CONTENT

S Supporting Information. Derivation of the chance-constrained solution and the mathematical solutions to Figure 3.This material is available free of charge via the Internet at http://pubs.acs.org.

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