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RESEARCH ARTICLE

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A decision-analytic approach to screening in chemical alternatives assessment

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Abstract

Material selection in the chemistry value chain involves consideration of many objectives, including cost, performance, health risk, and environmental impact. Alternatives assessment is an emerging tool for guiding complex decisions with respect to these goals. As a relatively new method, the process is not yet well developed, especially with respect to how trade-offs among objectives can be assessed accurately and inexpensively. Using paint strippers alternatives assessment as an illustrative example, we show how an established decision-analytic method, known as comparative screening, allows for a multistep process with gradually increasing information needs. Compared with existing methodological approaches, comparative screening instills flexible and consistent treatment of trade-offs. This is important because it maximizes the potential for a robust assessment while minimizing arduous data collection. Further, its use in the alternatives assessment process can support the selection of more sustainable materials.

KEYWORDS
alternatives assessment, comparative screening, decision analysis

1 | INTRODUCTION

Bringing a sustainable product to market requires decisions that consider stakeholders along the entire value chain. For example, material selection decisions at the product formulation stage take into account factors such as performance, cost, health risk, and environmental impact, as well as the ways in which consumers engage with environmentally friendly products. End users considering an environmentally friendly purchase face a complicated decision context (Shim, Shin, & Kwak, 2018), often responding with effort-reducing heuristics such as putting higher weight on environmental benefits only when product performance is considered as at least as good as the incumbent (Meyer, 2001). Product developers and procurement staff respond to these same trade-offs but often lack the tools to make a balanced decision (Byggeth & Hochschorner, 2006), especially when comparing both monetary and nonmonetary objectives (McWilliams, Parhankangas, Coupet, Welch, & Barnum, 2016). Limited understanding of how to handle these trade-offs is a source of confusion among sustainability stakeholders (Angus-Leppan, Benn, & Young, 2010). Thus, a structured approach is key to better decisions, improved understanding, and greater sustainability progress (Seager, 2008).

One place where structured decision-making may be especially useful is in the chemistry value chain. When it comes to selecting what chemical(s) to use, the decision stakes can be high. For many product manufacturers, it is critical to minimize the number of times they have to replace a chemical of concern because these substitutions can be expensive and disrupt commercialization schedules (Holder, Mazurkiewicz, Robertson, & Wray, 2013). For many brands and retailers, the conversation with suppliers has shifted from piecemeal chemical substitution to making systematic evaluation of alternative formulations a "fundamental component of product design" (McFadden, 2011). Alternatives assessment (AA) has emerged as a comparative approach to guide decision-making toward safer and more sustainable alternatives (Vesilind, Morgan, & Heine, 2010).

As a form of "whole product assessment" to inform chemical selection decisions, AA evaluates options for multiple attributes (e.g., cost, performance, hazard, and exposure) and can also consider life cycle metrics (Heine & Whittaker, 2018). Largely driven by markets or regulation, AAs have been performed for materials such as solder in consumer electronics (Malloy, Sinsheimer, Blake, & Linkov, 2013), formulated cleaning products (McFadden, 2011), and antifouling boat paint (Heine & Whittaker, 2018). Although practices have evolved for this relatively new method, much work remains to refine the AA process. Reviews of AA techniques have pointed to four broad areas that call for improvement (Jacobs, Malloy, Tickner, & Edwards, 2016; Malloy et al., 2017; National Research Council, 2014): (a) linking stakeholder preferences (e.g., hazard may be viewed as more important than cost) to alternatives ranking or selection, (b) assessing many attributes (i.e., energy use, performance, etc.), (c) treating uncertainty, and (d) generating an appropriate number of alternatives. As others have noted, the field of decision analysis has spent many decades developing methods to address these specific issues (Malloy et al., 2017). In this study, we investigate an area where decision analysis techniques have been underutilized: achieving consistency in the rules used for generating, screening, and selecting alternatives, especially with respect to hazard and exposure trade-offs.

2 | BACKGROUND

Many broad commonalities exist across AA methodologies (Tickner et al., 2018); after identifying the chemical of concern and formulating the purpose of the AA, users generate a list of potential alternatives, refine, and ultimately evaluate them in detail. Methods frequently diverge in the attributes considered as well as how and when to evaluate trade-offs among attributes (IC2, 2017). Some frameworks (e.g., Eliason and Morose, 2011) emphasize sequential pruning of alternatives, where the sequence of attributes (e.g., hazard, performance, etc.) used to reduce the pool of alternatives matches their importance to stakeholders. It is cognitively easier to compare alternatives one attribute at a time, and if an alternative is dropped at an early stage, then there is no need to collect data at later stages. Sequential frameworks, however, do not explicitly consider trade-offs among attributes and can prematurely eliminate options which would be preferred if a multiobjective approach was used.

In contrast, simultaneous frameworks (e.g., National Research Council [NRC], 2014) consider all attributes at once, allowing users to assess trade-offs among attributes. The degree to which a poor rating in one attribute can offset a high rating in another varies depending on the technique; this is referred to as compensation. For example, multiattribute utility theory (MAUT) allows for full compensation, whereas other techniques such as out-ranking allow for partial compensation (Malloy et al., 2013). Simultaneous frameworks may be less intuitive to a decision-maker, especially if a specific trade-off is viewed as unacceptable, and more time is likely to be spent assessing preferences and estimating all attributes for all alternatives.

More common than purely sequential or simultaneous frameworks are hybrid frameworks, which mix the two techniques. A typical hybrid framework uses sequential screens before a simultaneous evaluation. This allows for alternatives that score poorly on important attributes such as hazard and performance to be screened early, preventing needless collection of data on alternatives that are unlikely to be selected as a preferable alternative. The decision analysis literature (Keeney, 1980), however, has long cautioned that sequential screening should be done with care, especially if the attributes chosen for screening (a) are a means to achieve higher level objectives, (b) have similar levels of importance, or (c) cannot be assessed independently. If not implemented in a way that is consistent with the preferences that are represented in the simultaneous phase, then some alternatives may be prematurely screened.

This might be especially important for AA, which is traditionally focused on choosing an alternative chemical that is less hazardous than the existing baseline chemical in a product (Heine & Whittaker, 2018; Holder et al., 2013). Once the *less hazardous than baseline* threshold is met, the evaluation considers more complex interactions among hazard and exposure reduction, as well as other attributes. For this later stage analysis to be effective, a framework is needed to achieve alignment with selection protocols embedded in the threshold. In this study, we develop a comparative screening methodology that can account for a variety of preferences and reduces the likelihood of prematurely eliminating viable options. We apply the method to an illustrative example of methylene chloride AA for paint strippers. The results show how sensitive AA recommendations can be to screening methods, highlighting the need for robust and theoretically consistent approaches to addressing multiple attributes in an AA prescreening step.

3 | METHODS

Similar to Malloy et al. (2013) and other decision-analytic AAs, we use MAUT to rank alternatives given multiple attributes, such as risk and cost (Keeney & Raiffa, 1976). We refer to each alternative's overall desirability as its *utility* and the additive contribution from each attribute to *utility* as *attribute utility* (*i*). A standard assumption of MAUT is that a decision-maker or stakeholder can assess attributes independently of one another. For this work, our attributes are risk, performance, cost, and environmental impact, where risk is divided into hazard and exposure reduction subattributes (Figure 1). As a result, utility takes the form

$$U = k_{risk}u_{risk} + k_{perf}u_{perf} + k_{cost}u_{cost} + k_{env}u_{env}, \qquad (1)$$

where for attribute i, k_i are weights between 0 and 1 such that all k_i sum to 1, and u_i are attribute utilities between 0 (*worst*) and 100 (*best*). The value of weights assigns trade-off values to attributes. For example, if k_{risk} = 0.50 and k_{perf} = 0.25, then an increase in utility of 10 is

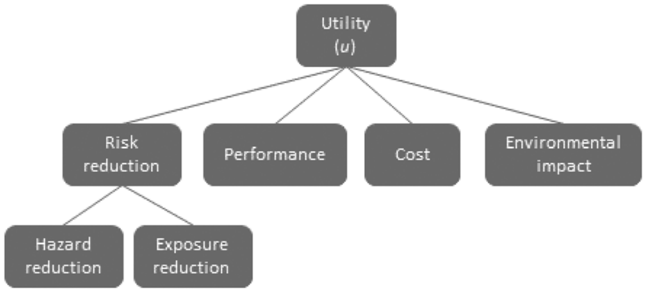

FIGURE 1 Relationship of attributes to overall utility of paint stripper alternatives

worth more for the risk attribute than the performance attribute: 5 versus 2.5. This means that in a situation where a stakeholder had to choose between an improvement in risk or performance (all other attributes staying the same), the stakeholder with these preferences would want the improvement in risk.

Given the emerging role of comparative and other types of exposure assessment in AA (NRC, 2014), we assume a flexible form for risk (Keeney, 1981) that accommodates a wide range of risk preferences:

$$u_{risk} = k_{haz}u_{haz} + k_{exp}u_{exp} + (1 - k_{haz} - k_{exp})u_{haz}u_{exp}. \tag{2}$$

For example, setting k_{haz} = k_{exp} = 0.5 puts equal weight hazard and exposure. It also represents a case where a stakeholder can assess each independently, as would any combination of k_{haz} and k_{exp} that sums to 1. For example, a stakeholder who is focused on hazard prevention and can assess hazard independent of exposure might have a value of k_{haz} close or equal to 1 and a value of k_{exp} close or equal to 0. Alternatively, hazard and exposure might not be valued independently in practice, as suggested by the use of comparative exposure assessments in some AA frameworks (NRC, 2014). In these cases, it is more likely that the sum of k_{haz} and k_{exp} will be less than one. This gives positive weight to the third term in Equation (2), which values alternatives in which both hazard and exposure are rated highly, effectively complementing one another. In the spirit of AA, it is unlikely a stakeholder would have preferences (k_{haz} + k_{exp} > 1) in which the third term is negative, as this would imply a penalty for an alternative with more desirable values of both hazard and exposure.

Although there are many ways to reduce the number of alternatives before a full analysis (Chen, Kilgour, & Hipel, 2008), we focus on a method that Keeney (1980) refers to as *comparative screening*. This technique approaches screening by first considering an alternative's desirability using a limited set of objectives. Alternatives are screened out if their desirability on the limited set of objectives is low enough that even a very high score on remaining unquantified objectives will not yield a competitive overall score. The limited set of screening objectives is chosen based on their importance to the analysis and how much effort is required to estimate each objective.

As an example, consider a decision where you are purchasing 1 of 20 cars based on cost, performance, color, and cargo capacity. If all the criteria for these attributes are easily quantifiable from manufacturer data or other sources, then one would proceed to consider the full criteria set when ranking alternatives. If one of the criteria, however, such as performance, requires costly tests or computer modeling to quantify, then there would be some benefit to reducing the pool of alternatives to a number that reduces the cost of gaining more information. In this case, one would rank the cars based on cost, color, and cargo capacity first. Cars would be screened out if their scores are low enough that even the highest score on performance would not make them competitive in the final analysis.

Thus, comparative screening can be generalized in two steps. The first step is to calculate the utility of all alternatives using only the attributes that have been quantified (U_S). The next step is to select the alternative with the highest utility score and subtract from it the highest possible contribution of the remaining unquantified attributes. For example, if an AA was screening based on risk and performance, this means selecting the highest utility score (U_S^+) based on risk and performance and then subtracting the highest possible utility scores for the cost and environmental impact attributes:

$$U_C = U_S^+(u_{safety}, u_{perf}) - \alpha\left(k_{cost}u_{cost}^+ + k_{env}u_{env}^+\right). \tag{3}$$

This leads to a cut off value U_C that can be used as a screen, where U_S for any alternative must be equal to or greater than U_C to be considered for further analysis. Note that in Equation (3), U_S^+ is the utility value of the highest ranking alternative when only considering risk and performance. The highest value for the unquantified attributes is usually assumed to be one (e.g., u_{env}^+ =1). Because this assumption leads to a relatively conservative screen (i.e., keeps more alternatives for full assessment), the parameter α can be adjusted to screen out more alternatives. By default α = 1, but if a less conservative screen is desired, then it can be set between 0 and 1. This might happen if there is a desire to limit trade-offs at the screening stage. For example, setting α = 0 indicates a preference for not allowing deficits in risk and performance to be offset by cost and environmental impact.

Another way of conceptualizing α is to rearrange Equation (3):

$$\alpha = \frac{U_S^+(u_{safety}, u_{perf}) - U_C}{k_{cost}u_{cost}^+ + k_{env}u_{env}^+}. \tag{4}$$

This equation relates the strictness of the screen to two factors. The numerator is the difference between the maximum and the lowest allowable utility achieved by the currently quantified attributes, in this case, risk and performance. The denominator is the highest possible utility achieved by all other attributes, in this case, cost and environmental impact. Thus, α is the fraction of remaining postscreen utility that may substitute for lower prescreen utility scores.

Assessment using MAUT requires specifying two preference types. One comprises different attribute levels, which is measured by attribute utility. The other is the relative importance of each attribute, as measured by the weights (k). Many techniques exist to assess MAUT decision-maker or stakeholder preferences (Clemen & Reilly, 2014). Given the illustrative nature of this study, we do not attempt to elicit preferences specific to the paint stripper problem or precisely calculate attribute values.

TABLE 1 Objective weights

Objective	Weight
Minimize risk	0.55
Maximize performance	0.15
Minimize cost	0.15
Minimize environmental impact	0.15

Attribute weights are informed by the weights elicited by Malloy et al. (2013). As shown in Table 1, this corresponds to risk receiving 0.55 of the weighting, whereas performance, cost, and environmental impact are weighted by 0.15, 0.15, and 0.15, respectively. In our analysis, exposure and hazard attribute weights (k_{haz} and k_{exp}) are not fixed; instead, we explore their influence on alternative ranking through sensitivity analysis.

TABLE 2 Hypothetical attribute

Formulation	Attribute				
	Hazard	Exposure	Performance	Cost	Environmental impact
A	0	75	100	100	50
B	0	100	100	75	75
C	50	25	100	100	100
D	50	100	75	0	100
E	50	100	100	50	75
F	75	100	50	50	75

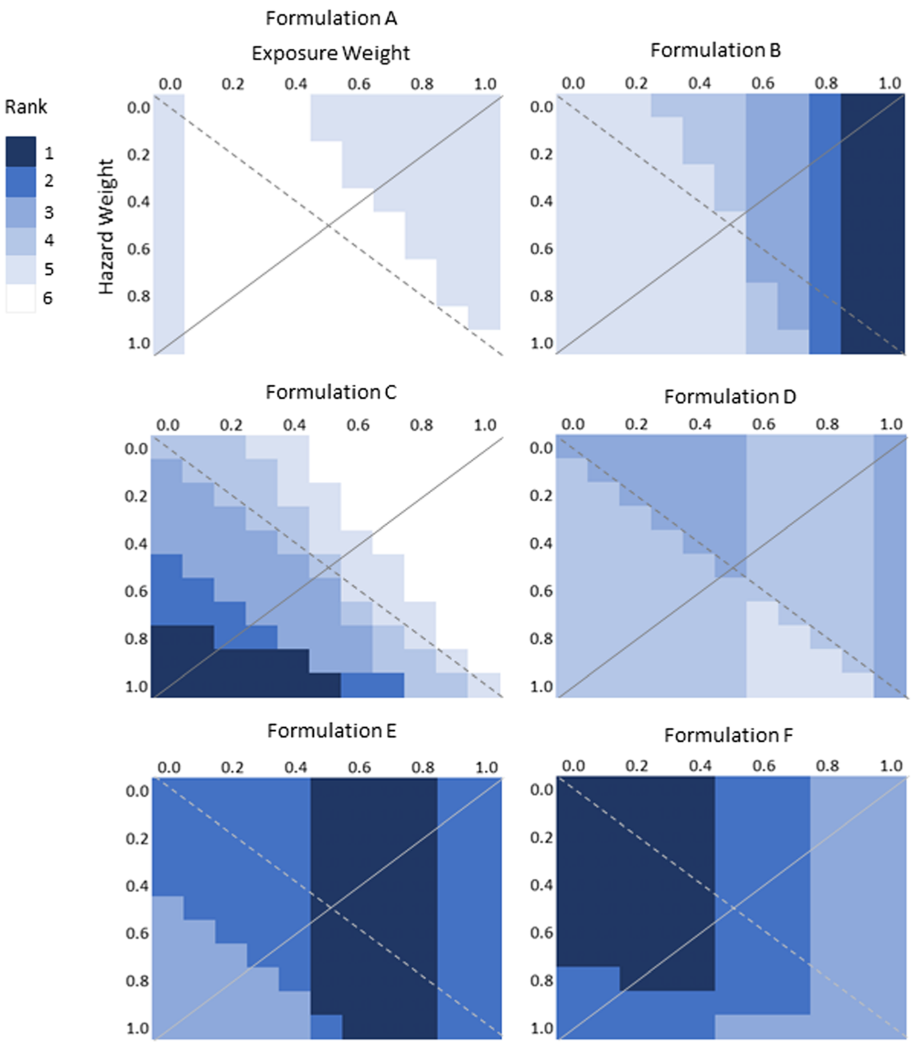

FIGURE 2 Alternative assessment results for each formulation. Each panel shows the rank of the alternative for different values of k_{haz} and k_{exp} from 0 to 1, indexed by increments of 0.1. Solid diagonal lines indicate where hazard and exposure preferences are independent, $k_{haz} + k_{exp} = 1$. Dashed diagonal lines indicate where hazard and exposure preferences are equal, $k_{haz} = k_{exp}$ [Colour figure can be viewed at wileyonlinelibrary.com]

To emphasize the illustrative nature of this study, hypothetical alternatives were created and assessed. Starting with the list of alternatives in Jacobs, Wang, and Rossi (2015), we use our background knowledge of paint strippers to create a small set of archetypal alternatives with quantified attribute utilities along a five-level scale (0, 25, 50, 75, and 100). As shown in Table 2, this allows for a manageable set of diverse alternatives to highlight the proposed methodology. In this setup, Formulation A is the baseline paint stripper; it is representative of a paint stripper formulation containing methylene chloride. Formulations B–F explore plausible formulations, including those with very different hazard and exposure profiles. For example, Formulation B scores lowest (worst) for hazard but highest (best) for exposure and has higher (better) values for other attributes. Alternatively, Formulation D represents a paint stripper with a high (better) environmental impact score and a relatively high risk score but lower (worse) performance and price scores.

4 | RESULTS

4.1 | MAUT model

Inputting the weights from Table 1 and the attribute utilities from Table 2 into MAUT functions of Equations (1) and (2) yields the results shown in Figure 2, where instead of choosing weights for hazard and exposure, we explore all possible combinations of weight values. This allows for a mapping of how different hazard and exposure preferences lead to different rankings of alternatives. In Figure 2, the solid diagonal lines indicate the boundary where hazard and exposure are independent, $k_{haz} + k_{exp} = 1$. To the left of this line, moving towards each graph's origin, are where preferences for hazard and exposure reduction are dependent and complementary, $k_{haz} + k_{exp} < 1$. As discussed earlier, if hazard and exposure preferences are in fact dependent, they would most likely be complementary. For the sake of exposition, we also show regions to the right of the solid diagonal lines, where hazard and exposure preferences are substitutes for each other, $k_{haz} + k_{exp} > 1$. Also delineated in Figure 2 are areas where either hazard or exposure reduction receives more weight: $k_{haz} > k_{exp}$ or $k_{haz} < k_{exp}$. These are separated by dashed diagonal lines, which indicate where hazard and exposure reduction have equal weighting: $k_{haz} = k_{exp}$.

Figure 2 shows that the baseline paint stripper Formulation A does not perform well compared with the hypothetical alternatives despite having the best possible scores on performance and cost. Formulation D also does not rank particularly well, with its highest ranking of 3 out of 6 occurring when relatively higher weight is put on exposure reduction. Both results are consistent with expectations of the MAUT model, as both formulations score

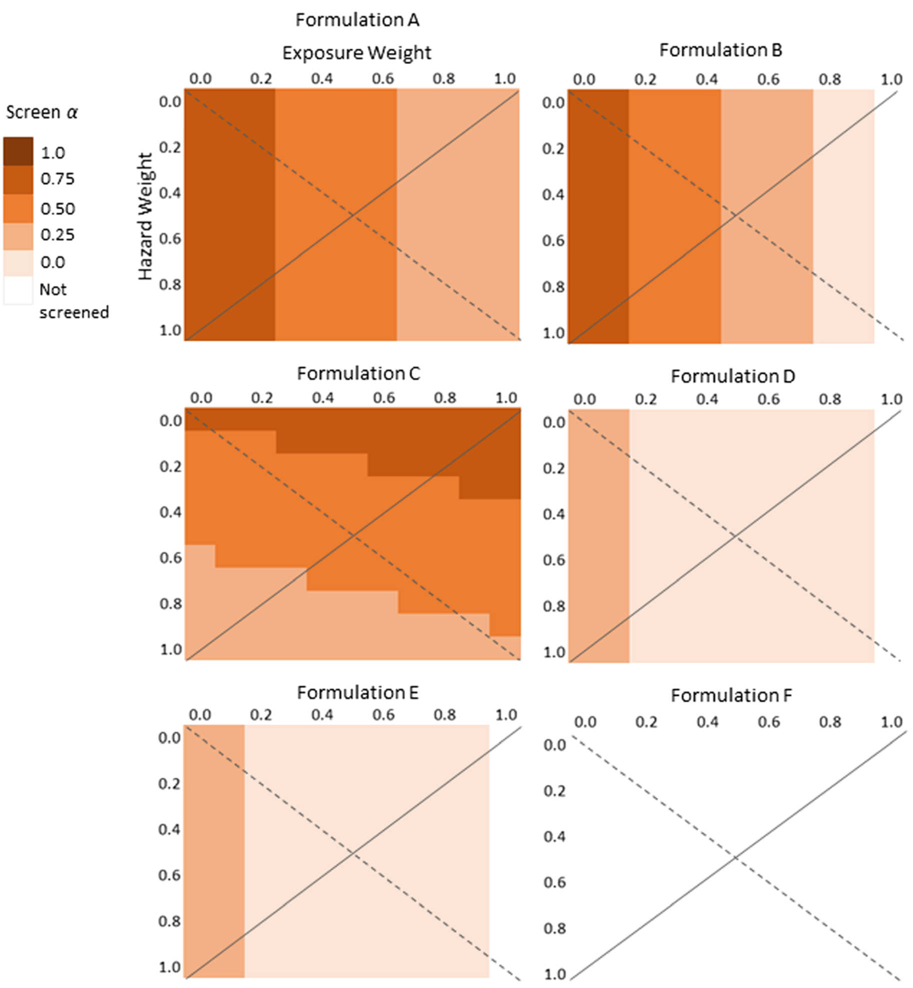

FIGURE 3 Alternatives that are dropped using a risk-only screen. Colormap shows the lowest value of α, in 0.25 increments, where an alternative passes the screen. For example, a value of 0.50 means that the alternative passed the screen for values of 0.75 and 1.0 but not for 0, 0.25, and 0.50. Solid diagonal lines indicate where hazard and exposure preferences are independent, $k_{haz} + k_{exp} = 1$. Dashed diagonal lines indicate where hazard and exposure preferences are equal, $k_{haz} = k_{exp}$ [Colour figure can be viewed at wileyonlinelibrary.com]

relatively higher (better) on exposure than hazard, but poorer on hazard reduction.

The remaining formulations (B, C, E, and F) all rank first but for different risk preferences. Formulation B has the lowest (worst) score for hazard, the highest scores for exposure and performance, and moderate scores for cost and environmental impact. As a result, it ranks best when exposure reduction is valued more than hazard reduction, $k_{exp} > k_{haz}$. As shown in Figure 2, its rank worsens as hazard reduction is valued more, despite its high scores on performance, cost, and environmental impact.

A reversed pattern is observed for Formulation C, where hazard reduction scores better than exposure reduction, with all other attributes scoring highly. It ranks highly when hazard reduction is valued more than exposure reduction. In contrast, Formulations E and F rank highly (first or second) over a wider range of preferences. Formulation E tends to rank higher when exposure reduction is more preferred and hazard and exposure are complementary, or when hazard and exposure reduction have similar levels of value and their reductions are substitutable.

Formulation F ranks first in areas where hazard and exposure reduction are complementary. Given that this formulation has relatively low (poor) scores for price and performance and high scores for hazard and exposure, it is expected that it would rank highly when risk preferences are complementary and not too extreme towards hazard or exposure reduction. Together, Formulations E and F rank first and second for about two-thirds of the hazard and exposure preference combinations in Figure 2, and in areas where they rank first and second, the difference in overall utility between the two is at most 6 units of utility. This is a relatively small difference given that the difference between the best and worst performing formulations can reach 30 units of utility.

4.2 | Screening model

As an illustrative example, this model indicates that MAUT-based AA can narrow down alternatives through simultaneous comparison. The result also makes the case that some sort of screening step would be useful so that resources are not spent on quantifying all attributes for lower scoring alternatives. As discussed earlier, our proposed comparative screening method is designed to be consistent with MAUT so that the same preferences are used throughout the entire AA.

For example, Figure 3 shows the result of using the risk attribute as a screen over the same risk preferences explored in Figure 2. In this demonstration, the strictness of the screen was adjusted from 0 to 1 in 0.25 increments. The darkest shade indicates that the formulation

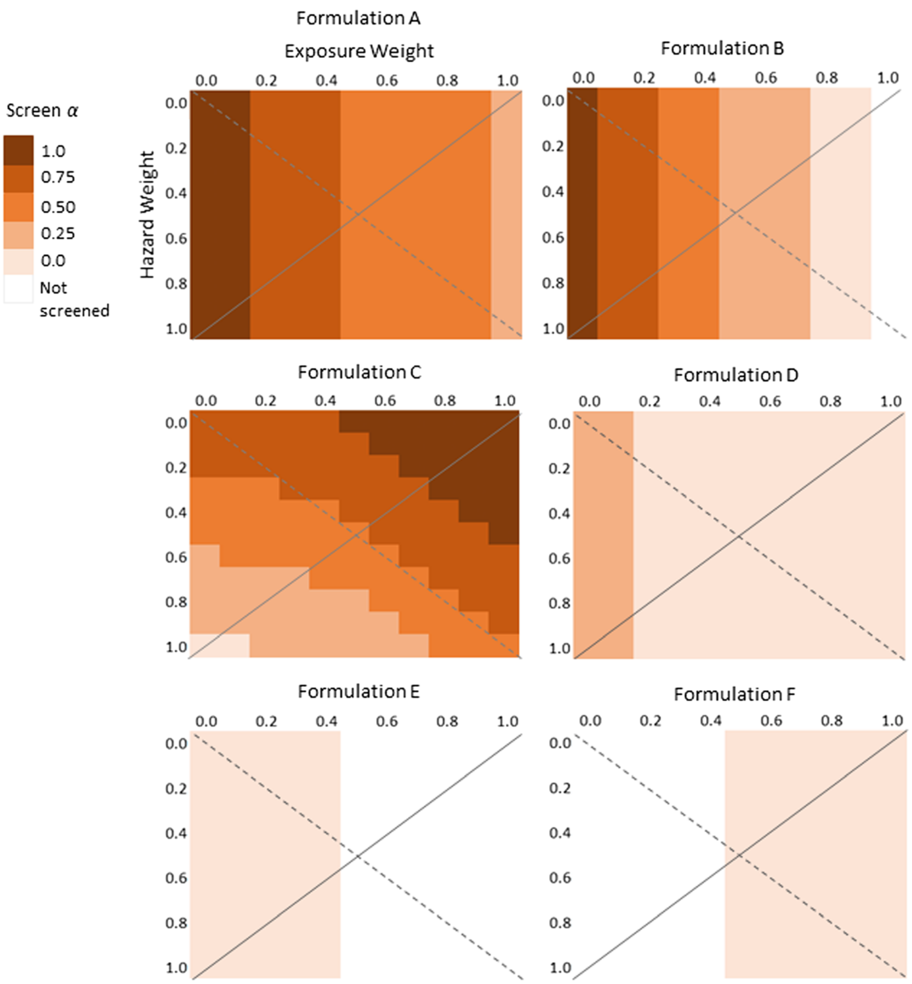

FIGURE 4 Alternatives that are dropped using a risk and performance screen. Colormap shows the lowest value of α, in 0.25 increments, where an alternative passes the screen. For example, a value of 0.50 means that the alternative passed the screen for values of 0.75 and 1.0 but not for 0, 0.25, and 0.50. Solid diagonal lines indicate where hazard and exposure preferences are independent, $k_{haz} + k_{exp} = 1$. Dashed diagonal lines indicate where hazard and exposure preferences are equal, $k_{haz} = k_{exp}$ [Colour figure can be viewed at wileyonlinelibrary.com]

would be screened out at α = 1, which allows full trade-off between risk and other attributes, and all other stricter screens. In contrast, white indicates that the formulation would not be screened out for any setting of α.

In this hypothetical case of screening, no formulations are screened out at α = 1, even when risk is entirely composed of hazard (k_{haz} = 1, k_{exp} = 0). Allowing less trade-off between risk and other attributes by setting α = 0.75 begins to screen out Formulations A and B for risk preferences that highly value hazard reduction over exposure reduction. This is expected as these two formulations have the lowest score on hazard. Setting α = 0.50 screens out Formulations A, B, and C, for most risk preferences in which $k_{haz} \geq k_{exp}$ and hazard and exposure are complementary. When $\alpha \leq 0.25$, which allows very little trade-off between risk and other attributes, Formulations D and E begin to be screened.

Once the screen reaches α = 0.25, which means that only one quarter of the utility deficit can be offset by nonrisk attributes, the screen begins removing alternatives that would rank highly. For example, the bottom-left corner of Formulation C is screened, even though this is also the area that is ranked first in the full simultaneous analysis (Figure 2). Similar problems occur for Formulation E when α = 0. Thus, care must be taken when choosing the strictness of the screen.

Using both risk and performance as a combination screen yields similar patterns to using only risk (Figure 4). However, depending on the specific risk preferences chosen, formulations A, B, and C are screened out for α = 1. This occurs because a perfect utility score for risk and performance combined would be 70, whereas a perfect score for just risk is 55. There is less attribute utility left to compensate, so the screen can be more lenient. As with the risk-only screen, the risk and performance screen does not begin prematurely drop alternatives until α = 0.25.

5 | CONCLUSIONS

Our results show that risk preferences strongly affect alternative ranking and screen properties, as indicated in Figures 3 and 4. If hazard and exposure are assumed as independent when in fact stakeholders view them to be dependent, then there is a chance that the AA results will produce suboptimal results and subsequent decisions. Although decision aids frequently include assumptions that deviate from reality in many ways, these deviations should be well understood and communicated to users or be inconsequential to the results.

We also show that it is possible to construct multiattribute screens, as opposed to relying on single attributes to sequentially screen alternatives. This result shows decision makers should consider the theoretical consistency of all AA steps so that the decision aid correctly represents objectives the stakeholder(s) view as important. Assuring consistency between AA steps, as illustrated above, is an important step toward adapting decision science methods "to fit the practical needs of AA" (Tickner et al., 2018).

Comparative screening reduces the likelihood of inadvertently filtering out alternatives that could rank highly in a simultaneous analysis by allowing for consistent stakeholder preferences across both the screening and full assessment steps. Although our results are based on an illustrative example of paint stripper alternatives, the hypothetical alternatives are representative enough to provide evidence for the efficacy of comparative screening when coupled with MAUT for AA. Further research in this direction should seek to test the reproducibility of our results with other chemicals, explore the importance of screening with frameworks other than MAUT, and elicit diverse stakeholders' preferences, objectives, and decision heuristics.

As AA becomes more widely used throughout the market place and in regulatory settings, it is critical to design these assessments to provide accurate results while maximizing inclusivity and minimizing administrative burden. Our screening methodology shows that many assessments can occur rapidly by using existing information, creating a workable solution for stakeholders. We encourage additional exploration of decision analysis principles within AA to further increase its utility as a structured, holistic approach supporting the selection of more sustainable materials.

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