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# Facilitating the transition to sustainable green chemistry

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Sustainable green chemistry depends on technically feasible, cost-effective and socially acceptable decisions by regulators, industry and the wider community. The discipline needs to embrace a new suite of tools and train proponents in their use. We propose a set of tools that will bridge the gap between technical feasibility and efficiency on one hand, and social preferences and values on the other. We argue that they are indispensable in the next generation of regulators and chemistry industry proponents.

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## Introduction

Chemicals have improved life expectancy, human health and material living standards, even though many are toxic and accumulate in the environment [1,2]. Sustainable green chemistry [3,4] aspires to expose the human population and environment to effective chemicals safely and equitably, accounting for the needs of current and future generations [5]. Chemical regulatory policy in many jurisdictions has shifted towards closer interactions between industry and the wider community [6,7], articulated by government regulatory agencies who typically focus on the assessment, approval and auditing of pollutants and toxicants [7–9]. Chemical regulatory agencies have a social mandate, in effect, to keep the human population and the environment 'safe' while at the same time assisting society to reap the benefits of chemicals.

Despite the international adoption of the *UN Sustainable Development Goals* in 2015 [7] countervailing pressures to innovate for profit and market advantage remain, precipitating standards that fail to protect human populations from serious harm [10] and recent initiatives to dismantle environmental regulations [11,12]. Even when clear directives exist, motivational bias and local priorities may seriously impede progress [13]. Without appropriate incentives, reform of the chemical industry ultimately will fail.

Sustainable chemistry requires a new social configuration, a more holistic approach [7] involving institutions, social practices and technological infrastructure [9]. To achieve this, it needs tools to support engagement between industry, regulators and the wider community. This study outlines briefly some of the regulatory commonalities in different jurisdictions, identifying gaps in risk management procedures. Finally, it outlines briefly a suite of engagement tools including stakeholder maps, argument maps, values hierarchies, structured decision making and market incentives. Their application will encourage more transparent, inclusive and fairer regulatory decisions, help industry to prepare for new challenges, and the public to exercise the power of consumer choice and to engage in risk management; all essential precursors to a more holistic, sustainable chemistry.

## Regulation and trust

Regulators build conceptual models of transport, fate and effects to estimate the effects on people and the environment when chemicals are used as prescribed, extrapolating exposure-response tests and other evidence to determine 'safe' circumstances. Technical experts evaluate the safety of proposals and identify risks to human populations, species and ecosystem functions [14–18]. All jurisdictions use some form of screening-level risk assessment in which regulatory scientists assess whether a proposal is 'safe' or requires more detailed and thorough (and costly) evaluation [19]. They also depend to some degree on data supplied by proponents.

Decisions invariably involve values [20] and are susceptible to a raft of uncertainties including social context, prevailing attitudes, motivational bias and the values and preferences of the assessors themselves that typically are not transparently handled [21–24] and may lead to inconsistent decisions [10,25]. Regulatory risk assessments focus on the impacts of individual chemicals, ignoring exposure to multiple pollutants, their interactions [11] and effects on non-target wildlife [26–28].

The resolution of these problems does not lie in simple restrictions, because most of these chemicals have beneficial uses that may exceed their costs. Nevertheless, such issues invoke questions of the equity of the distribution of the risks, the assessment of trade-offs among competing social and environmental values, and the creation of appropriate incentives to ensure the long-term viability of sustainable policies. These topics have been barely explored in the literature on sustainable chemistry (but see Ref. [29]).

Reibstein [11] discussed ethical sustainable chemistry and raised the issues of industry participation, governance, fairness, accountability, transparency, reputational risk and trust [22,30,31]. Many applied scientists aspire to having their work contribute to policy decisions. Many public servants regularly seek unfettered, unbiased and well-informed scientific input [24]. However, despite their aligned aspirations, there remain significant gaps between the kinds of information that scientists provide and the kinds of inputs that public servants find useful [32,33]. Usable science most often arises when researchers and policy makers work together, iterating problem formulation and solutions [34], engendering reciprocity and personal interactions [35,36]. Effective contributions are enhanced by mutual respect and understanding, timely responses, pragmatic solutions, and an awareness of the frailties of scientists in providing policy advice [37–40]. Policy decisions may take decades to develop and are the product of many social and political factors [41]. Sustainable chemistry requires a suite of tools to identify and examine trade-offs among competing values, create appropriate incentives and develop strategies to serve net social benefit and the equitable distribution of risk and reward.

## Tools for sustainable green chemistry

A broad range of tools may serve sustainable chemistry by closing the gaps between scientists, regulators, industry and the wider community [20,42]. They include stakeholder and argument maps, values hierarchies, structured decision making and market design. To illustrate these tools, we posit a new hypothetical chemical, *X*. In this scenario, analogues of *X* have been used in manufacturing and food production for many years without known harmful effects. Laboratory tests do not reveal deleterious effects on test organisms. The chemical is proposed for use in a novel setting, namely, controlling weeds in agricultural crops, and is likely to find its way into waterways. Its release is politically contentious.

### Inclusivity: stakeholder mapping

When contemplating effective social engagement, the question arises, who should be involved? Stakeholders may be defined as those who may influence a decision or be affected by its outcomes (see Figure 1), including future generations who may be represented by proxy stakeholders such as NGOs [23,43].

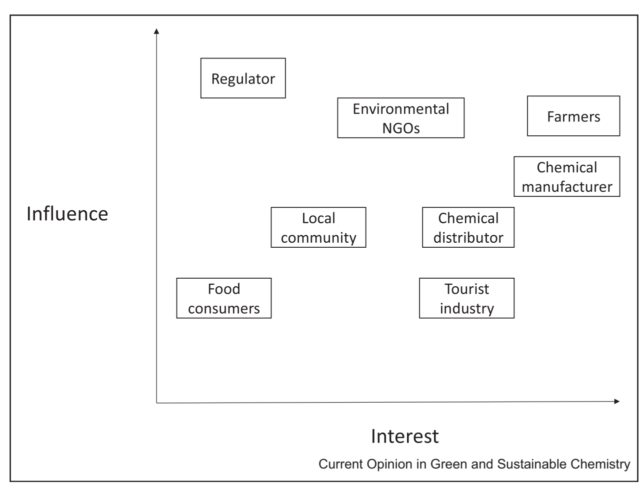
The boundaries of a problem are determined by the interests of stakeholders, including those not present [44] or unwilling to participate [30]. Marginalised groups increase the legitimacy of outcomes, but also increase the complexity of deliberation [45]. Stakeholder maps help to identify stakeholders and to position them relative to a decision. Usually, stakeholder maps place concerned individuals and organisations in a space defined by their influence over and their interest in the decision. The map is developed iteratively with stakeholders, assisting community and agency participants to discuss the decision and their involvement in it, providing insights into local networks, and clarifying issues of trust and organisational/agency influence [46].

### Improving transparency: argument maps

Often, the evidence supporting regulatory decisions is not clearly linked to the reasons for or against the decision, potentially creating distrust. Argument maps provide a mechanism to make regulatory decisions more transparent (see Figure 2).

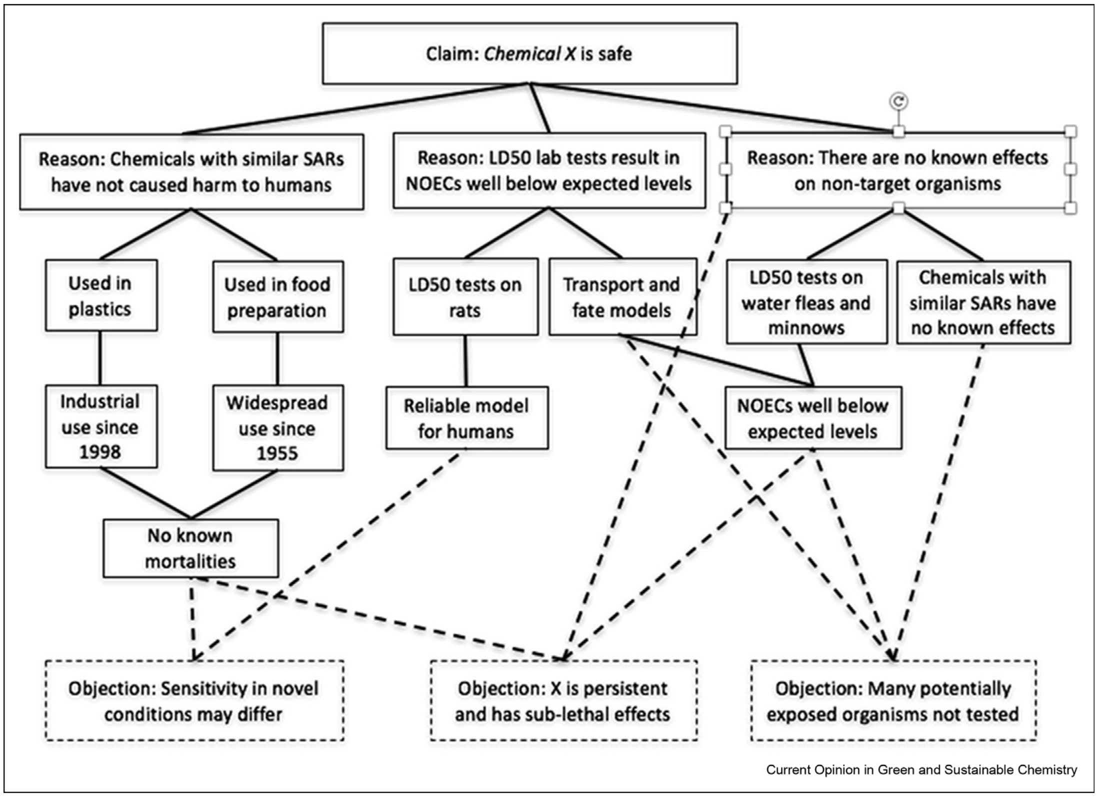
A claim is supported by reasons, evidence and sources [47]. For instance, experts use scientific understanding of a chemical's transport, fate, exposures and modes of action to evaluate whether it is safe, or can be used with restrictions. An argument map can represent unambiguously the reasons why the proposition (the chemical is safe) could be true (supporting reasons) or false (objections) [48] (Figure 2). Representing reasoning in this way leads naturally to positing counterfactuals, that is, lines of reasoning that lead to the opposite claim (i.e.,

**Figure 1**




Example of a stakeholder map for the hypothetical scenario of the decision to release Chemical *X*.

Figure 2




Argument map showing the reasons and evidence for the claim that a hypothetical Chemical *X* is safe enough to be used with regulatory constraints, together with objections to the claim. SARs are Structure Activity Relationships. LD50 tests refer to experiments to determine the concentration at which 50% of test organisms die within 96 h of exposure. NOECs are No Observed Effect Concentrations, exposures at which there was no discernible (typically, no statistically significant) effects occur on test organisms within 96 h. Sources of evidence would also normally be included. Many other kinds of evidence and potential objections may have been included.

that the chemical is in fact unsafe). These are usually represented as 'objections', in this example, that the chemical is persistent, has sub-lethal effects, some exposure pathways may be novel, and many non-target organisms have not been tested. Each objection links to pieces of evidence or to the reasons themselves (see Figure 3).

There is no formal way of assigning a weight to each of the reasons, lines of evidence, or objections. Assessors must form a subjective opinion on the likelihood that the chemical is safe or should be regulated.

## Dealing with value judgements: values hierarchies

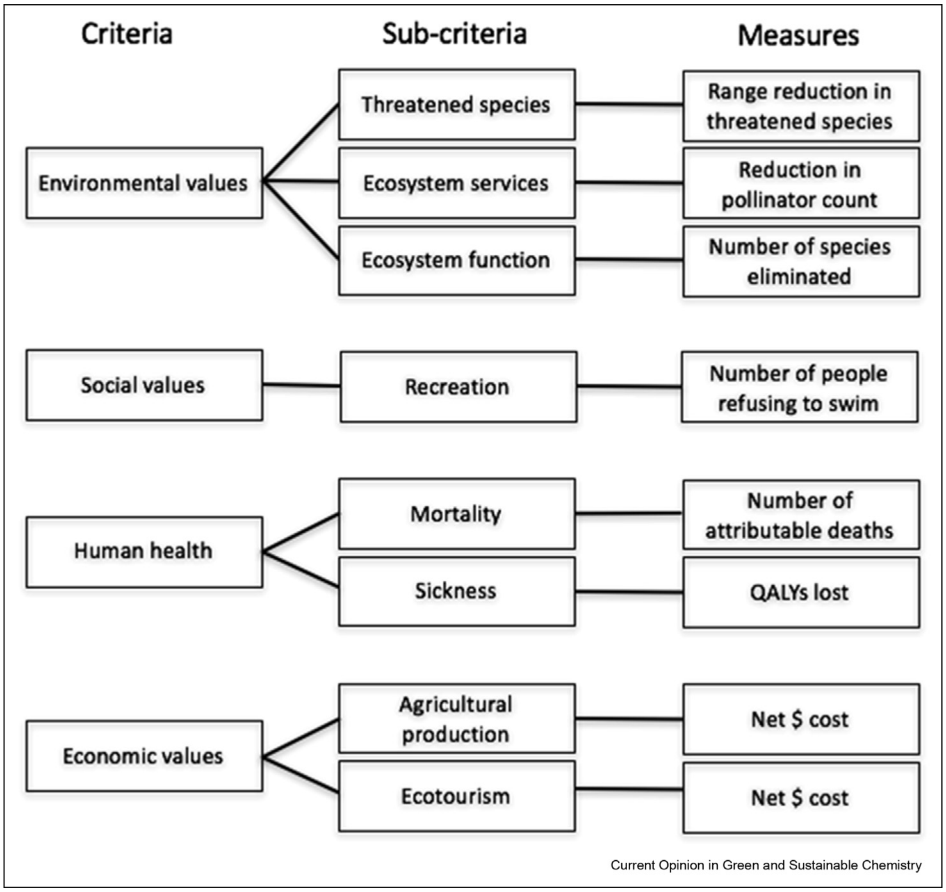
Assessments may entrain estimates of effects on things as disparate as transitory effects on the health of children, increased likelihoods of cancer in adults, impairment of the function of freshwater invertebrates and constraints on the trade of agricultural products that reduce employment opportunities. Trade-offs inevitably involve values, and risk analysts trained in conventional chemistry are poorly prepared to deal with them. Values hierarchies (objectives hierarchies) assimilate the things that people care about, and that might be affected by a chemical. Each sub-criterion should be accompanied by an unambiguous and operationally feasible measure (a direct measure, a proxy or a constructed scale) (see Figure 3) [20,49]. If properly constructed, they help decision makers and stakeholders to discriminate ends (fundamental objectives, the things people really care about) from the means of obtaining them.

The objectives hierarchy is used to order thinking about important attributes (criteria), to ensure no important elements are overlooked, that criteria are meaningful and decomposable, and to avoid redundancy in judgements [49–51]. It provides a mechanism for integrating different ways of perceiving or understanding environmental and social issues [9,52].

## Understanding trade-offs: structured decision making

One of the mantras of sustainable green chemistry is to negotiate decisions that are consistent with the values

**Figure 3**




Values hierarchy for hypothetical Chemical *X*. The concerns (objections) identified in the argument map have been distilled into 4 main criteria, namely environmental, social, human health and economic criteria, and 8 sub-criteria.

and aspirations of all stakeholders [5]. Structured decision analysis tools provide the link between risk assessment and social preferences. The first steps, as articulated above, are to identify stakeholders, create a values hierarchy and decide on relevant measures. Next, identify management alternatives (options) and score (estimate) the criteria under each action. Finally, specify weights for criteria and subcriteria, aggregate the scores, and evaluate the sensitivity of outcomes to weights and scores. Alternatively, participants may discuss the tradeoffs and identify a consensus position that accommodates minimally satisfactory outcomes for all participants [20].

Structured decision making can be effective for complex problems that include monetary and non-monetary values [53], eliciting judgements about the relative importance of personal, organisational or societal values [54,55]. Ideally, facilitated interactions between stakeholders can be used to document and discuss the diversity of opinions [56]. Sensitivity analysis can identify where scores, weights or approaches to aggregation have a critical effect. Insensitive criteria such as ecotourism and human health effects in Table 1 which vary little over the alternative actions may be disregarded. Participants may develop alternative actions that better satisfy their objectives. Uncertainty information is a crucial element, allowing stakeholders to evaluate their attitude to risk, their willingness to take risks to achieve better outcomes, versus their propensity to settle for more modest, but more assured outcomes [57]. Thus, farmers may support restricted release because it avoids potential losses (Table 1).

## Understanding motivation and acceptance: market design

Most regulators depend on information supplied by proponents, potentially creating disincentives to find problems, or to disclose them once they are discovered. The regulation of hypothetical Chemical *X* provides an example. Expected human health impacts, measured as quality-adjusted life years (QALYs [58]), vary little over the three potential actions, from 1 to 2 QALYs per 100,000 people exposed. These data are likely extrapolated from the results of tests conducted by the company. If the company fails to find important or significant

**Table 1**

**Hypothetical decision table for six of the sub-criteria identified in the values hierarchy above, for each of three potential decision actions (no release, restricted release, and unrestricted release). The role of scientists in this process is to estimate the consequences and uncertainties for each of the criteria under each of the decision options. The impacts measure the added effects of release, compared to the existing baseline. The uncertainties are 95% confidence intervals, or their Bayesian equivalents.**

| Sub-criteria | Measures | No release | Restricted release | Unrestricted release |
|---|---|---|---|---|
| Threatened species | Range reduction | 3.0 ± 1 $km^2$ | 3.5 ± 1 $km^2$ | 12.5 ± 10 $km^2$ |
| Ecosystem function | # species eliminated | 2 ± 5 | 7 ± 5 | 50 ± 30 |
| Recreation | # people not swimming | 0 ± 10 | 15 ± 10 | 20 ± 10 |
| Human health | QALYs # per 100,000 | 1 ± 2 | 1 ± 2 | 2 ± 2 |
| Agricultural production | Net $ (million) | 200 ± 50 | 800 ± 50 | 900 ± 300 |
| Ecotourism | Net $ (million) | 20 ± 5 | 19 ± 5 | 19 ± 5 |

effects, regulation will be less stringent. Even in the absence of deliberate deception, this incentive may exacerbate confirmation bias. Likewise, the absence of information about effects on non-target species is taken to suggest that there are no unacceptable effects.

Bier and Lin [59] pointed out that the number of firms choosing not to comply with environmental standards will grow as standards become more stringent. Companies have the opportunity and the motive to provide inaccurate and favourably biased information. Regulators and the wider community have reason to doubt the integrity of the information provided by companies. Wagner (1997, in Ref. [59]) claimed, for example, that inadequate testing and/or lack of disclosure were at least partly responsible for significant harm from tobacco, the Dalkon Shield, and asbestos. Sustainable green chemistry relies on establishing conditions in which companies disclose fully and look proactively and thoroughly for potential problems. Ideally, it will be in their self-interest to do so.

Game-theorists have established that market design and regulatory policy can deal with perverse incentives effectively. For example, self-reporting procedures with penalty reductions may encourage auditing and disclosure [60]. Bier and Lin [59] illustrated how relaxed restrictions for companies that disclose breaches can encourage honest reporting. Zhao et al. [61] outlined government policies that result in holistic supervision of supply chains to reduce carbon emissions. Such models may be used to evaluate strategic behaviours and behavioural styles, and assess the importance of factors such as willingness to make strategic concessions, risk attitude, and knowledge of other parties' preferences, leading to policy options that encourage fair and efficient sustainable behaviour [62–64].

## Discussion

The tools outlined here fill some important gaps in conventional chemical regulatory procedures. Importantly, they target those elements that are most important to sustainable green chemistry, namely equitable accounting of the full diversity of social values and preferences, building transparency and trust, and creating environments which encourage industry, regulators and the wider community to cooperate.

These approaches provide a key additional dimension that can support improved decision-making, one that is ignored on most conventional regulatory environments. Specifically, decision makers can evaluate both the expected (most likely) outcome of a decision, and the robustness of decisions to uncertainty. A decision option that promises a higher return might be declined in favour of an alternative with lower expected value but lesser uncertainty of outcome [65,66]. Similarly, a decision that is optimal from the social (central) planner's perspective might be declined in favour of a solution that is socially stable [67]. Such decision making under uncertainty can only be undertaken if the extent of uncertainty associated with alternatives is understood and communicated clearly, and those affected have the opportunity to consider their attitude to risk taking.

The tools outlined here have limitations. It can be difficult to reconcile opinions about cause and effect, and data can be ambiguous or unavailable. It can be difficult to construct objectives hierarchies, to ensure all factors are included, that weights are broadly accepted and that means and ends have not been confused. Structured decision analysis, if applied naively, can lead to anchoring, reinforcement of entrenched positions or personal value judgements. The procedures above may deal adequately with the needs of the current generation, but deal only indirectly with those of future generations. Above, we advocate stakeholder maps, argument maps and structured decision making to support the elicitation of consequences assessments. But these tools will be effective in the long run only if market forces and incentives are designed to encourage participation and cooperation.

## Conflict of interest

Nothing declared.

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